TOWARDS STRUCTURALLY INTEGRATED DESIGN ACROSS TRADITIONAL CHEMICAL PROCESS BOUNDARIES

A Thesis

by

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ABSTRACT

The purpose of this work is to establish the concept of structural integration for the efficient use of equipment in chemical processes via an approach that systematically provides synergetic opportunities towards structurally integrated design across traditional process boundaries. The systematic methodology is developed in three phases. The problem formulation considers the process flow diagram of standalone plants and the structural integration opportunities as the input and the output to the procedure respectively. The first phase includes the representation of the input in a numerical framework. The second phase sets-up the desired output by identifying possible opportunities that can be utilized in chemical processes. Then, the third phase deliberates the generation of logical steps that appropriately identify the opportunities from the given input by implementing algorithm flowcharts of various synergy types. This developed approach is validated by conducting an illustrative example. Two standalone plants are simulated, subjected to heat integration, and economically evaluated. The application of the developed approach identified synergetic opportunities that are then used in the synthesis of a structurally integrated plant. The illustrative example results in capital cost savings up to 31% and an overall annualized cost savings up to 18.5% constrained by same production quality and quantity. These savings shall justify the main motivation of the study that is reduction in capital investment of chemical processes towards a more efficient design.

DEDICATION

To my mother

ACKNOWLEDGMENTS

First and foremost, all praise is to Allah the Almighty

I would like to extend my gratitude to my main advisor, Prof Patrick Linke, who wisely taught me that hard work should be objective of which an un-selective hard work may result in dilution of core idea. His long-term vision in research used to enlighten my steps towards my research goals. His respectful and transparent attitude during this research played an essential role in maintaining a productive and a safe research environment. Thanks to my committee members, Prof Mahmoud El-Halwagi, who was generous and pleasant during the communications. Regardless of him being part of my research committee, his assistance overseas via his self-explanatory text books is undeniable. Thanks to Porf Hamid Parsaei for his kind collaboration. I cannot leave any stage of success in research before admitting that a great favor goes back to my first teacher in research, Dr Mert Atilhan. Respect and gratitude to Dr Easa Ismail Al-Musleh for his undeniable efforts and rigorous supervision during my BSc senior year which have made me ready for advanced tasks in higher education of my field of specialization. Thanks to my family, my backbone, for their unconditional love and support, warm prayers to succeed, and patience on my frequent absence. Thanks to Qatar National Research Fund for hosting me in their research community and placing their trust in my potential. Thanks to Mr Ahmad Al-Nouss for being available whenever a guide is needed for the use of simulation software. Thanks to the faculty of the Chemical Engineering program at TAMUQ. Thanks to my colleagues and friends for their help and support.

NOMENCLATURE

$\mathcal{M}$	Molecular Weight, grams/moles
$\mathcal{F}_{mass}$	Mass Flow Rate, kg/hr
$\mathcal{F}_{mole}$	Molar Flow Rate, kmole/hr
AcOH	Acetic Acid
MeOAc	Methyl Acetate
MeOH	Methanol
EtOH	Ethanol
MeI	Methyl Iodide
P	Set of plants
E_P	Set of equipment in plant p
C	Set of components
ACETI-01*	Acetic Acid
METHA-01*	Methanol
ACETATE*	Methyl Acetate
DIMET-01*	Dimethyl Ether
IODIDE*	Methyl Iodide
HYDRO-01*	Hydrogen
ETHAN-01*	Ethanol
PROPI-01*	Propionic Acid
LITHI-01*	Lithium Iodide

- Units are mentioned as they appear here unless otherwise stated
- Alternative use of nomenclature and the meaning in the text maybe encountered
- Symbol*: Notations are used to describe components in simulation and may be found in simulation related data tables

CONTRIBUTORS AND FUNDING SOURCES

Contributors

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TABLE OF CONTENTS

LIST OF TABLES

Page

LIST OF FIGURES

Page

CHAPTER I

INTRODUCTION AND LITERATURE REVIEW

I.1 INTRODUCTION

The chemical process design problem raised as an issue concurrently with the evolvement of the industrial implementation of chemical processes which is subject to development until present time, and expected to keep undergoing development in the future towards an overall better process performance. Before addressing the approaches towards developing the process design, it is essential to consider the ultimate objectives of designing a chemical process. The design problem can be seen from two perspectives. The first one is the pure technical aspect that deals with the nature of the chemical process, or in other words, the aspect that tries to answer the question of how to get a particular chemical specie produced in a given quality. This aspect is mostly associated with the production of new technologies or production of new species without much of attention towards the economics nor how much intensive is the design towards accomplishing this target. The other aspect is the aspect the looks into the chemical process as an investment. This aspect of the design problem tries to answer the question of how the design can improve the economic profile of a chemical process. Hereby, it can be seen that, up to a good extent, the second aspect seems to start only after the first one is satisfied for a given process. That is why by viewing the history of chemical process engineering design it can be observed that its objective was undergoing addition of specifications as a function of the developed stage of the discipline. In principle, the basic goal behind implementing chemical industries is to get chemicals produced upon demand, dealing with the first aspect. With this aim, the industrial applications of chemical processes started in the 18th century. Since that time, the process design techniques have been developing, taking care of the second aspect.

Hereby, for the general purpose of this research, the discussion can move deeper towards the second aspect. Indeed, by looking into the chemical plant from the investment point of view, this production needs to be carried out with respect to the profitability equation. Profit is simply sales minus costs associated with the process. It needs to carry an overall positive value to justify the economics of investing in a given chemical plant. Moving deeper into the aspects of profitability equation, sales variable considers factors that may not be directly related to the technical aspect of chemical engineering but rather with a market analysis that determines the demand and the supply. Thus, the contribution of a chemical engineer to enhance the profitability result is limited to the cost aspect. The cost of a chemical process is actually a summation of different cost parameters that are considered in a chemical industry. The four main factors that contribute directly in determining the cost are capital cost, operating cost, utility cost, and raw material cost. By classifying the cost into categories, it becomes easier to define the possible contribution of chemical engineering towards enhancing the profitability of the plant. It can be seen that the capital cost has more of concern about the core design of the process and equipment, the utility cost is mainly concerned about the energy system I the process, the raw material deals with, for example but not limited to, the selection of the technology, while the operating cost results from the prior selections.

According to the preceding arguments, the development of chemical process that aims to directly enhance the economic profile of the process, should end-up objecting one or more of these cost variables. In order to link the cost to the nature of the chemical process, the original factors that lead to minimize these are actually directly and explicitly defined. They are the well-established seven themes of chemical process research and development identified by Keller and Brayan (2000), briefly, reductions in capital inventory, energy use, better environmental performance, more attention to quality, enhance process flexibility, reduction in raw material and

emphasis on process safety. [1] These themes are to be further discussed in this text in later sections. By bringing back the economic profile of a chemical plant to the main objectives that deal directly with the nature of the process, the attempts towards enhancing the industrial performance can be easily defined and identified.

To basically achieve the most general objective of this work, namely enhance process performance, the attempts that developed in the literature are briefly stated here with more elaboration in later sections. A number of attempts that have the motivation to enhance the performance of the chemical process are developed. For example, but not limited to, Process integration approaches (mass, heat, property), process optimizations (including superstructure optimization), and going to a wider view to consider total sites and eco-industrial parks. These attempts have been successfully contributing in enhancing the performance, although form different approaches. One main observation about these attempts that their function starts only from a defined flowsheet. For example, heat integration considers a well-defined plant prior of setting the targets of utility saving by matching the cooling and heating streams. Also optimization, although it might influence the operating conditions, selection of equipment type, its view aims to enhance the performance of the process by an enclosed view into particular operating units. Moving from these attempts to the eco-industrial park and total sites, it can be observed that the great achievements by these approaches deal with the process as a black box. Thus, these attempts achieve the target of enhancing the chemical process performance by being concerned about factors other than the core structure of the process design.

Hereby, the problem statement of this research can be explicitly defined as follows: this research is concerned about enhancing the chemical process performance via developing a more efficient process design that deals directly with the overall process structure in the context of crossing the traditional chemical process boundaries. In other words, this research aims to develop a systematic approach to manipulate the process structure with respect to the structure of other processes, aiming to end up with an overall more efficient process structure than the summation of the original ones.

By moving to a more dedicated section of the introduction that is concerned about defining the main terminologies to be used throughout the research, the main principles and definitions are to be addressed. Since the research is mainly objecting the process design as the variable to reach that target of enhancing the process performance of process design and parameters should be clearly identified and stated. First, the parameters of process synthesis and design are to be briefly addressed. Second, the terminologies used throughout the text to help the reader in following the approach are to be clearly stated. Starting with the first, because this research aims and is directed towards the core structure of the process, the main principles in process synthesis need to be identified. Identifying the parameters of the main principle is essential in the process synthesis improvement reproach for two main factors. The first, is sort out the factors that are used to accomplish synthesizing a chemical process, while the other is to sort out the way of implementing the available factors. The first is important can be introduced. The other factor is important in order to identify whether the actual need is not with identifying new factors but rather adopting new techniques in using them due to a deficiency of the original ways. By stating this argument, the text can move more precisely towards the discipline of process synthesis. The process design approach has been a subject to modifications and development to basically enhance production

and or improve its quality. The accomplishment of this objective takes into account the fundamental principles of chemical engineering, making up the process synthesis discipline. Basically, the definition of a process is achieving a given target by sequential operations or at least one operation. [2] A given objective may be accomplished by multiple ways or more precisely multiple designs of units' arrangement and selection in the process. Enhancing the quality of a given material or coming up with a new one is the target of process design which represent the inventory action of making ideas to be converted into process. [3] The building blocks of the process are the equipment which are divided into two main categories. The first one is the Proprietary equipment, (pumps, compressors, filters, centrifuges, and dryers). [4] The other category is the Nonproprietary equipment (reactors, distillation columns, and heat exchangers). [4] The nonproprietary equipment participates to represent the phases in the hierarchy of traditional process design. Hereby, the building blocks (design variable and tools) and the overall definition of process design are defined. The second point takes into consideration defining the terminologies that are to be used throughout the text. Because the approach is toward having a better performance of chemical processes by looking into enhancing the structure after crossing the traditional chemical process boundaries, the approach is motivated towards having a greater benefit by combined system out of individual system than the total summation of the individual systems. This simply is the principle of the term "synergy". In the context of chemical systems, looking into the plants in a structurally combined manner is believed to result in benefits that are greater than dealing with the summation of the stand-alone plants. A stand-alone plant term is used frequently in this text, referring to a chemical plant that functions within its own boundaries without interaction with external plants. It is important to note that the important aspect of this research is appreciating the system in the perspective of number of plants, and hence having an optimized,

heat integrated etc. stand-alone plant does not conflict with the overall objective of this study. The important aspect is the interaction of the plants across its original defined boundaries. Also, it is important to note that a chemical plant is dedicated for a particular production. The production maybe more than one chemical species, however it is limited to a well-defined set of species within its stand-alone boundaries. Finally, the term structural integration is used, introducing the overall approach and summarizing it in this term. It refers the integration approach that is developed in this work which can be defined as a systematic approach establishes the fundamentals to integrate the structure/process flow diagram across process boundaries towards a more efficient process design.

I.2 LITERATURE REVIEW

The basic objective of conducting a literature review is to educate the researcher about the available and developed topics within the same field, and to help in further enhancing the focus toward the study. Furthermore, it highlights the need and implies to the significance of the study of interest in the context of the developed literature that has one or more objective in common. From the researcher perspective, it does enhance the maturity of the researcher about the field of specialization. For the current study, the literature that is reviewed is to be classified into categories to enhance the understanding of the aspect that the current research calls for. Before this, the aspect that this research considers is re-defined here to match the context of the categories of the literature review section. This study has the main objective of enhancing the process performance with a more specific target that is directed towards reduction in the cost associated with the structure of the process (mainly capital cost); the variable that the study manipulates is the process structure flow and design (the process flow diagram elements) structure of other standalone processes.

Despite the fact that attempting to enhance process performance represents a busy research topic in the field of chemical engineering design and development, it is not the original objective for the design activity, but it was evolved as a response to these targets. However, only until few decades back, the focus behind the design activity started to expand toward the efficient use of energy. Number of approaches were developed starting from 1977 to respond to the needs from the societal and industrial sectors. [5] These needs raised due to the industrial emissions of the greenhouse gases, waste water and material, and the excessive use of energy. Thus, sustainable design via heat and mass integration is a subject of interest. Thus, the following questions are to be answered here: are there attempts that aim to enhance the chemical process performance? What

are the main objectives of these attempts in the context of the seven themes for process engineering research and development? Are there attempts that aim for the same objective but with an attention towards the structure design of the process? What are the available techniques to perform process synthesis? If any, does any of the objectives of the attempt can be approved systematically? Now, these question are to be answered in the context of the representation of the hierarchical nature of chemical process. Also, it is used to show the classifications of these contributions. In the literature, attempts to enhance the process performance can be classified into categories: enhance the performance in the context of the stand-alone plant and from the context of participation of number of plants. The other classification of these attempts is concerned with the type of the attempt itself whether it deals with the energy systems, capital investment, environmental protection etc. These classifications are to be addressed in the context of the plant design established phases. The onion diagram representation is known as the onion diagram. The onion diagram is originally presented by Linhoff et. all (1982) [6]. This diagram is reproduced and shown in Figure I-1*.

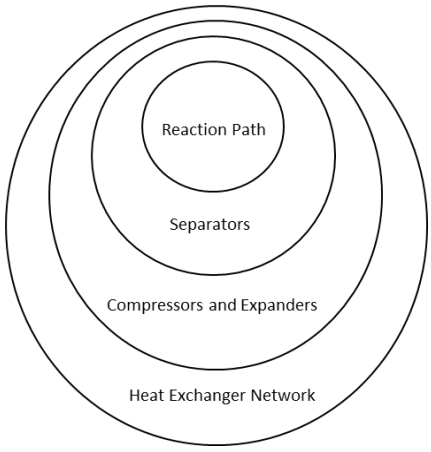


Figure I-1: Onion diagram representation*

*Reprinted with permission from User guide on Process Integration for the efficient use of energy. by Linhoff, B, Townsend, D, Boland, D., Hweitt, G., Thomas, B., Guy, A., and Marsland, R., 1982. Copyright [1982] by The institute of chemical engineers.

An updated representation that is to be used to move forward is the one available by Smith and Linhoff (1988) [7] and reporduced in this strudy as shown in Figure I.2. All phases of process design development mentioned earlier can be illustrated in one diagram, including the phase of the interest in this study of this research. The illustration of the traditional hierarchy of process synthesis and design can be used as a base to appropriately explain how the implementation of these targets can be accomplished. For Figure I-2, as shown, its starts with the reactor (R), in the core, followed by the separation layer (S), and then by the Heat Recovery system (H) or heat management, and lastly by the utility System (U). The two inner layers, reactor and separations, define the material balance envelope. Basic structure of the flowsheet process synthesis while the outer layers of Heat Recovery and Utility Systems deal with the heat balance envelope both are objects of a design activity that was called process integration. [3] Starting with the core inner layers, namely the reactors and separation systems (which fully define the functionality of the process), the literature review on the developed approaches in their regard is found to be limited to the basic techniques to address the process synthesis target.

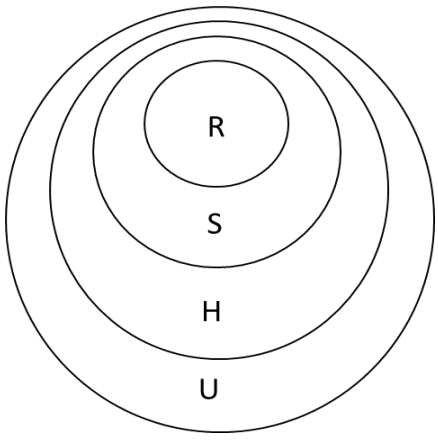


Figure I-2: Onion diagram representation by [7]

Design text books such as, but not limited to Smith, 2005, [8] Sinnott and Towler, 2012 [4], Seider, Seader, and Lewin, 2004 [9], Vogel, 2005, [10] provide information about steps, techniques, improvement to accomplish process synthesis and design. Up to this level, process synthesis is being supplied with guides from three main sources. The traditional approaches to improve process are briefly brainstorming (generation of multiple scenarios and select the most convenient one), adopting and evolving, and Heuristics [11]. One conclusion can be made on these approaches as stated by El-Halwagi [11] that despite their great assistance to the development of the discipline, they lack approaching solutions in a systematic manner. One approach that address the design problem systematically is optimization. It deals with the core and outer layers with an overall objective of enhancing the process performance. Process optimization is simply defined by setting an objective function, i.e. cost/energy use for a given design variable, say operating conditions, while being constraint by product specification for example. Other optimization techniques and systematic approaches that is motivated to enhance and develop the core, with respect to the process boundaries is Process Intensification. It is a systematic approach towards sustainable production for generating options for process development. [12] By this, the core layer vision development took into considerations as well development with respect to a number participating plants. Such example is superstructure optimization by looking into optimizing one unit in the context of multiple plants or processes. Some examples on this attempt, include optimizing the reaction-separation [13]. Other attempt takes into consideration reaction-reaction network [14]. By this, the literature on development of process synthesis is done, and to move into the outer layers, namely the Heat Management and Recovery layer. The first attempts towards enhancing the process performance within this layer is addressed by Linhoff et al [6] with later developed advances on the technology. The heat integration approach contributed in a step-change in process

advancement that is directly linked to minimization of utility cost and use. Thus, it does not contribute in the core layer. Then, Mass integration, which may be exemplified by El-Halwagi and Manousiouthakis [15] in the synthesis of Mass exchange network. These approaches extended from considering stand-alone plants to include system of plants as the example of EIP. EIP can be defined as the design and execution of integration of waste treatment, material for exchange and disgorge in a shared infrastructure of many processes which may belong to different organizations. [16] Material of integration considered by-products, Carbon dioxide, and water. By this, the contribution of EIP has been concerned by integrating the two our layers, in addition to waste material, by-product, and water integration.

Hereby, by viewing the history of chemical process development, with special attention to the attempts that aim to enhance the chemical process performance, eventually, it may be noticed that most of these attempts are applicable only after the design problem of the core technology is defined, dealing with the core elements of the process as rigid elements. For example, but not limited to, approaches such as process integration (mass and energy), eco-industrial parks, total sites, etc. develop the performance by starting from the defined core structure and more importantly, their application does not influence the design of the core structure of the process.

CHAPTER II

ESTABLISHMENT OF STRUCTURAL INTEGRATION CONCEPT

The conceptual understanding to structural integration towards a more efficient process design can be illustrated by viewing its contribution in the context of developed advances in enhancing chemical process performance. Basically, integration is the act of combination. Thus, the very basic understanding of structural integration can be appreciated as a combined structure. In the context of chemical process, the structure of a given process is defined by its inter-connecting units or what is the so called process flow diagram. Thus, a combined structure of n number of processes may refer to combined flow diagrams of the processes. The essence of structural integration concept can be seen via the definition of the term synergy: the interaction of elements that when combined produce a total effect that is greater than the sum of the individual element. Conceptually, the combination of unit operations in chemical processes is expected to result in benefits. This due to the expected elimination, alteration of tasks and/or fully/partially share of tasks within the chemical process. Fundamentally, by looking back into the seven themes for chemical process development, direct benefits in the themes of capital cost, and process flexibility may be anticipated. This conceptual understanding can be better appreciated by properly fitting it in the context of the developed advances in chemical process performance. This can be done from two perspectives. The first one, is a direct comparison with the developed integration categories, namely, heat and mass integration. The aim of comparison is not to differentiate among categories but rather to enhance the understanding of the range and the direction of the new concept. The second perspective, is to evaluate the concept with respect to the attempts that aimed to enhance the process performance across chemical process boundaries, namely, Eco-industrial

parks. Classification of developed integration categories with respect to the seven themes is illustrated in Table II-1 along with the expected benefits of Structural Integration.

Table II-1: Chemical Process Integration with respect to the Seven Themes for Chemical Process Research Development [1]

Direction	Mass Integration	Heat Integration	Structural Integration
Reduction in raw material cost	🟡	🟡	🔵
Reduction in capital investment	🟡	🟡🔴	🟢
Energy use reduction	🔵🟡	🟢	🟡
Ever greater emphasis on process safety	🔵	🔵	🔵🟡🔴
Increased attention to quality	🔵🟡	🟡	🔵🟡
Better environmental performance	🟢	🟢	🔵🟡🔴
Increase in process flexibility and reduction in inventory	🟡	🔴	🟢

Key:

🟢 Main Objective 🔵 Indirect Benefit 🔴 Negative 🟡 Neutral/depend on the case

As shown in the table, the main objective of Structural Integration may serve as a complementary aspect to other developed approaches towards an overall enhancement to process

performance. This is because it covers an uncovered aspect before, and it misses aspects that is significantly addressed before. Overall, a complementary use of the three integration categories may serve as the overwhelming target towards overall enhancement of process performance. It is worth mentioning that in the classifications of benefits, the outcome of some themes is classified with the extreme negative, indirect benefit at the same time since structural integration outcomes depends on the use of identified integration synergies what makes the performance of the design dependent on the resulted design itself.

The other perspective that is considered to appreciate the contribution of Structural Integration is to directly fit it within the context of developed attempts that work on the principle of crossing the process boundaries. In this exercise, the concept of Eco-industrial parks is used as an example. To properly illustrate this, the terminology used in the literature review chapter is re-used here to validate the contribution, namely, the onion diagram. In simple words, one onion represents one standalone plant. As shown in Figure II-1, two stand-alone plants are completely independent. This independency includes independent process reactors, R, independent separation and recycle systems, S, independent Heat recovery system, H, and independent utility system, U. This independency is further illustrated by the red-dashed process boundaries.

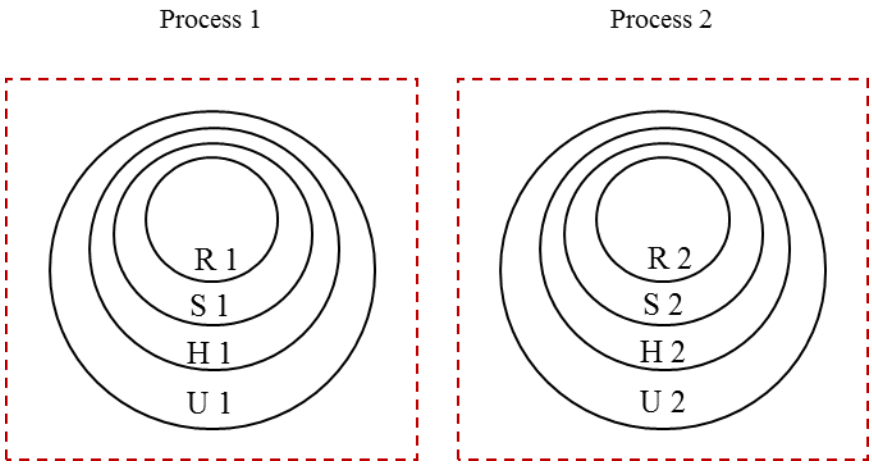


Figure II-1: Stand-alone process with complete independency

Attempts to cross the process boundaries that are clearly represented by Figure II-2 include Eco-industrial parks. As previously addressed in the literature review section, eco industrial parks attempted to cross process boundaries with water and energy systems. These systems are part of heat-recovery and utility outer layers involved in the simple onion diagram. Thus, the contribution of eco-industrial parks to cross process boundaries, for example, to cross the boundaries of processes is to integrate the heat recovery system across the two processes as well as the utility system. It is important to emphasize that this attempt keeps the original rigid boundaries around the core of each of the processes. Thus, the original structure of basic units I process flow diagram is considered as rigid elements from the perspective of eco-industrial park research. This contribution is illustrated in Figure II-3.

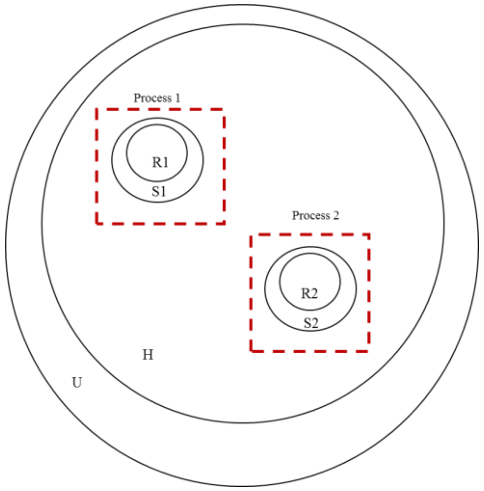


Figure II-2: Eco-industrial Park Participation in enhancing process performance by crossing process boundaries partially

The main concept that structural integration calls for is the integration of the core structure of the process. The core structure that traditionally used to be defined as a property of a give process since it determines the production and the nature of the process. This core structure has already illustrated by the simple onion diagram to represent the core layers, namely, reactions, followed by separation and recycle layers. In other words, the main elements of process flow-sheet. It is worth mentioning that an integration of separation may be done independently, simultaneously, and/or in order with the reactor layer as illustrated in advance sections of this work. The integration of the core layers that represents the contribution of this research for chemical process performance enhancement is illustrated in Figure II-3.

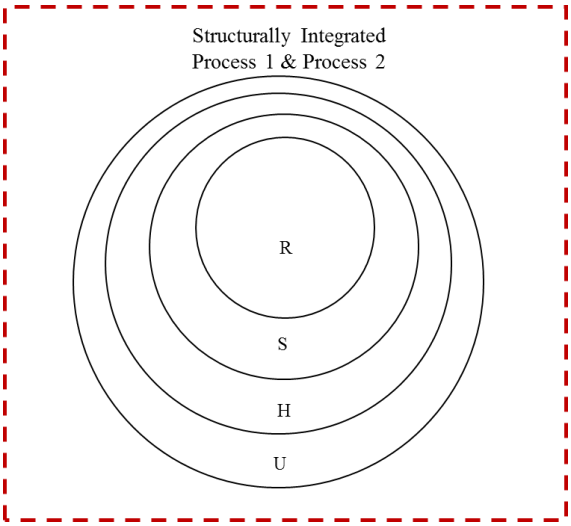


Figure II-3: The contribution of this research in establishing structural integration concept

As shown in figure II-3, all boundaries that are originally presented in the original system of process 1 and process 2 are essentially crossed by structural integration. By accomplishing a structure integrated design, the participating process may be appreciated as one process that can be presented in one onion diagram, representing the original hierarchy of process design phases.

After illustrating the conceptual approach of structural integration, it essential to provide an understanding about the range of applicability and acceptancy of the approach. In other words, the constraints of structural integration should be defined. In this context, the constraints maybe defined as the limit of the execution of the structural integration act. These constraints are listed below:

1. Production Type.al chemical specie that is being produced in the original process. i.e. the act

2. Production Capacity. i.e. the amount that is produced in the original process.
3. Production quality. i.e. mass/mole/volume concentration, impurity concentrations etc.
4. Any other specification and/or constrain that must be satisfied by the original process in independence of the above three constraints. i.e. particular use of solvent for considerations other than the production.

Structural integration may result in retrofitting existing plant, however, because it brings plants physically together, it is mostly expected to result in re-implementation.

CHAPTER III

SYSTEMATIC APPROACH DEVELOPMENT

III.1 INTRODUCTION

One factor that differentiates an established principle in process design from a single-successfully designed process is the approach towards the identified solutions. The structural integrated design problem that is introduced in this research is approached systematically. The essence of approaching the design problem systematically is represented by the assurance of the reproducibility of the solution and the ability to visualize the identified solution in the context of multiple alternatives to eventually consider it as a scientific contribution.

This section provides a comprehensive picture about the phases of the systematic approach development needed to tackle the problem of this research. It shows how the developed general approach is implemented into synergies of interest. Synthesizing the method or the approach follows three main phases: propose the desired output, determine the needed and/or available input, and generate steps/procedure to properly transform the available input to the desired output. Each of these phases has sub-classification. The input of the systematic approach of this work is sub-classified into two phases of formulation and representation, the desired output is sub-classified into types and routes, while the generation of the steps/procedure is sub classified into set of rules and specifications. Then, after the synthesis phase is fully defined by the generation of Algorithm to appropriately transform the input into the desired output by instructive steps. More specifically, the input and the output determine the range of the method. Between the input and the output sequential execution of steps is followed. These steps are represented in an algorithm. For the formulation phase, the input information is classified into sets. One set includes the participating processes in the structural integration, a second set includes the operating units/equipment

involved in every element of the first set, namely, set of processes, and a third set gathers chemical species involved in all processes without repetition. Ultimately, the input is represented in an encoded process flowsheet that is to be transformed into an output of integration opportunities of synergies as shown in Figure III-1.

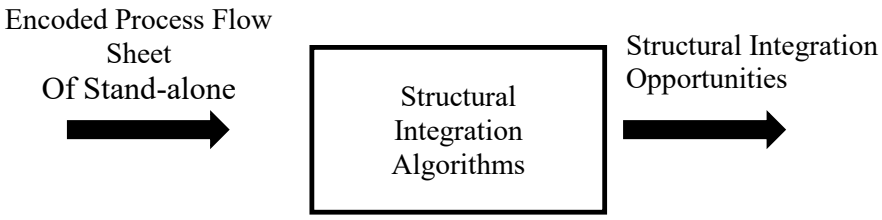


Figure III-1: Overall Systematic Procedure Schematic Representation

III.2 PROCEDURE INPUT: PRIMARY SPECIFICATIONS

III.1.1 Introduction

The input to the procedure is the process flowsheet for number of plants. The essential elements for the integration must be identified, formulated, and represented to provide the proper input format to the systematic procedure. Because the procedure is systematic, it needs to generalize the input data to handle multiple examples and cases. First it is essential to determine what is exactly needed from a given process flow diagram to have the sufficient information required for structural integration across plants. This need can be identified by the following reasoning. This integration type is concerned about:

1. Integrating across process boundaries (Number of Plants) ….

2. The process building blocks (operating units/equipment per one plant) …

3. By function of the units. (Function is defined by the flow of components around units)

The above three points that together restate the aim of this work provide the break-down of the major participants in the integration, namely the plants, equipment per plant, and the flow of components. The following two sub-sections provide the consequent steps towards adjusting the identified parameters of the plants to be ultimately classified as data input. These sub-sections represent the formulation of these data that is followed by representation to properly prepare the input ports within the procedure to be general enough to handle multiple example towards systematic approach.

III.1.2 Formulation

The first phase in adjusting the input framework is the classification of the important parameters identified earlier. This is defined as the formulation phase. The formulation phase is

concerned about classifying the elements identified in the preceding paragraph in a proper manner with an objective to ability of navigating among the classified elements for procedure search. The following classification is followed:

1. The first category is the highest order set of plants. This set is donated to as P set.
2. The second category is the lower order set that is the set of equipment of every plant. This set is donated to as E_P. This category includes only the following equipment type
    a. Reactors
    b. Separators
    c. Compressors
3. The last category is the category of chemical species or components. The components are classified in set donated to as C set. Note that this set is a global set since it accounts for one chemical specie once. i.e. if a chemical specie exists in multiple plants, multiple units it is counted once in the C set. Every element in this set is assigned to a unique number that does not change. Neither order nor distribution is important unless otherwise specified.

The following example is conducted as a hypothetical example for the purpose of illustration of the application of the sets in a given system of chemical plants:

Hypothetical Example 1: application of sets into a system of plant

Figure III-2 shows a simple-hypothetical plant flow diagram that consists of a liquid feed the is pumped and then heated along with a gas feed that is compressed in two stages and heated prior to fed to the reactor, then the reactor effluent is expanded for two steps purification units. Figure III-3 shows another hypothetical plant flow diagram, consisting of one-stage compression gas feed that is pre-heated with a pumped liquid feed that is alps preheated to enter the reactor,

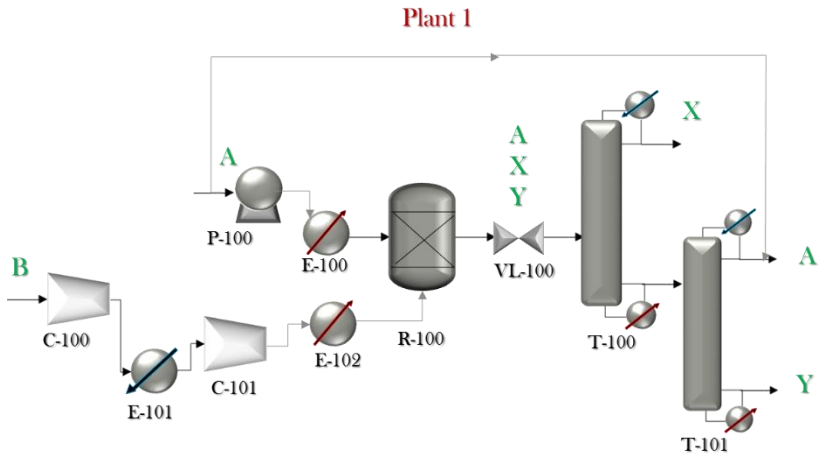


Figure III-2: Schematic Diagram of Plant 1, Hypothetical Example 1

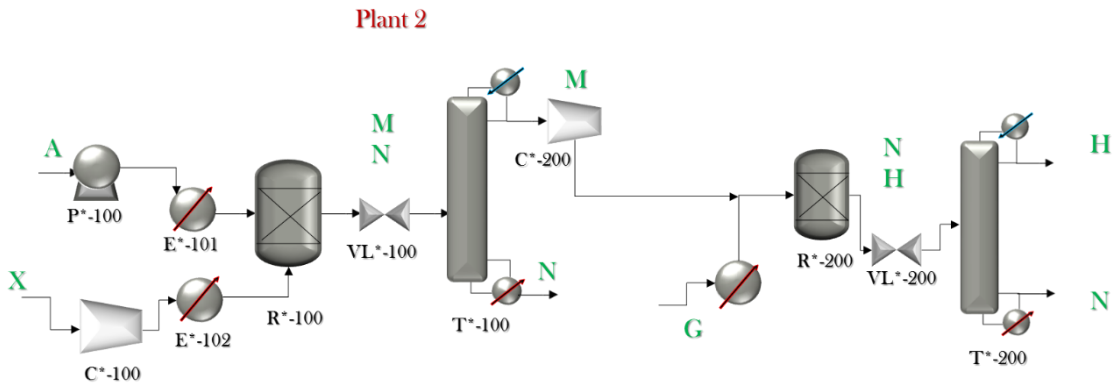


Figure III-3: Schematic Diagram of Plant 2, Hypothetical Example 2

then the expanded effluent enters a purification column of where the top product is compressed and enter another reactor of which its effluent in expanded and then purified in a single step. The equipment of plant 2 are donated by star to differentiate them from plant 1 equipment. These two plants represent the system of plants that is to be subjected to structure integration. Thus, according

to the formulated input, their parameters, plant, equipment, and components need to be classified into sets.

Solution:

Plants: Plant 1 and Plant 2 (total 2)

Equipment: C-100, C-101, C*-100, R-100, R*-101, R*-100, T*100, T-100, T-101 (total 9)

Components: (total 8)

Thus,

$P = \{1,2\}$

$E_{P=1} = \{1,2,3,4,5\}$

$E_{P=2} = \{1,2,3,4,5,6\}$

$C = \{1,2,3,4,5,6,7,8\}$

Where A=1, B=2, X=3, M=4, N=5, Y=6, G=7, H=8

By the end of this section, it should be noted that the development of this section is the classification into sets. However, the numbering manner within every et is subject to change depending on the coming development phases of the systematic approach.

III.1.3 Representation

The categorized elements that participate to define the system of participating plants in the activity of structural integration should be accessible via one representation. This representation should properly organize the important information of these elements for further use in the

procedure of synergy search. One suggested representation is representing the elements on the Cartesian coordinate since the number of sets is ultimately three. Figure III-4 shows a three dimensional representation pf n=3 plants on the Cartesian coordinate, classifying P on the z axis. similarly, the y would represent the Equipment set while the x would represent the Component set.

By now, there is still a need to properly fit the three dimensions into one useful representation that may be accessible to extract information from the system of interest. One suggested representation is the use of matrixes. A matrix that has two dimensions would have y number of columns and x

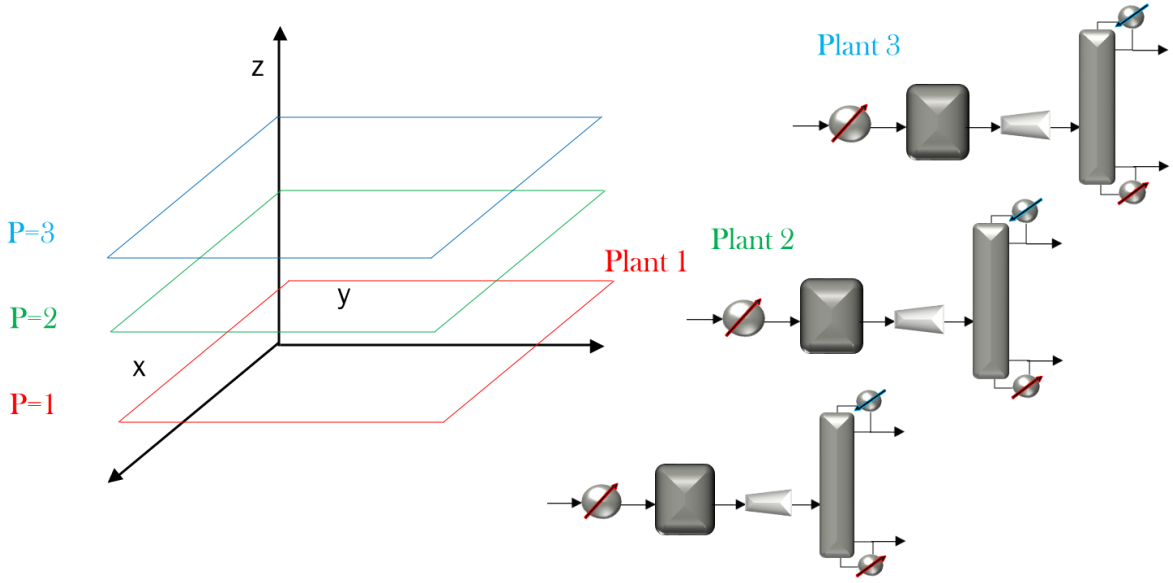


Figure III-4: Representation of n=3 plants by the use of Cartesian coordinate

number of rows, while the third dimension would be z number of two dimensional matrixes. Hence, it can be said that a two-dimensional matrix may represent one process or plant that has y number of equipment (represented by E set) and has an x number of component represented by C

set), while the system acquires z number of plants (represented by z dimension). The following general conditions hold for the use of this representation:

1. P set contains the number of plants with increasing order for positive integers only. P sets represents the number of z elements that is the number of two-dimensional
2. matrixes. For example, if the system has 4 plants, it would acquire 7 two-dimensional matrixes. Neither order nor distribution of the participating plants is important.
3. E set contains the number of equipment of every plant (of every element of z P set). The type of equipment needed for data extraction and the numerical representation is as follows:
    a. The type of equipment should be determined
    b. Every type of equipment that needs to be distinguished from another type acquires a unique numerical representation among positive integer set of real numbers.
4. C set contains the set of chemical species participate in the system. As illustrated earlier, this set is rigid in all plants (in all elements f P set that is represented by two-dimensional matrix)

Hypothetical Example 2: illustration of the matrix representation for encoding the process flow diagram

Figures III-2 and III-3 shown earlier need to be encoded by the use of the matrix representation explained earlier. The following rules can be used for encoding:

i. Consider only reactors, distillation columns and compressors as equipment.

ii. Use the rows of the two-dimensional matrix to represent the C set elements while use the column to represent the E set element

iii. To classify the different type of E elements into the columns, consider the following:
    a. Use multiples of 3 for reactors
    b. Use even positive integers AND non-multiple of 3 for compressors
    c. Use odd positive integers AND non-multiple of 3 for distillation columns

iv. Keep the matrix empty but just use highlights for illustration of the classification of the sets into the matrix.

Solution:

First, the sets to be generated. By the use of the solution of hypothetical example 1, the sets are known. The number of rows in every matrix is fixed since it represents the number of elements in C set that is a global set. The number of columns of every two dimensional matrix

varies depending on the number of equipment and type of equipment being used in every plant (since every plant is determined by two dimensional matrix).

Thus, the following hold for matrix representation of every plant:

1. The number of rows of every matrix equals to the number of elements in C set, that is identified earlier (check hypothetical example 1) as 8 elements.
2. The number of two-dimensional matrixes equals to two that is the number of elements in P sets (participating plants)
3. The number of columns for plant 1 (shown in Figure III-5) is as the following
    a. Reactors hold column number 3 only (one reactor, starting with 3 that is the least number of the multiple of 3 set)
    b. Distillation columns hold columns 1 and 5 that are the least two odd positive integers AND non-multiple of 3.
    c. Compressors hold columns 2 and 4 that are the least two even positive integers AND non-multiple of 3.
4. The number of columns for plant 1 (shown in Figure III-6) is as the following
    a. Reactors hold column number 3 and 6 (one reactor, starting with 3 that is the least number of the multiple of 3 set and ending with 6 that is the second least number of the multiple of 3 set)
    b. Distillation columns hold columns 1 and 5 that are the least two odd positive integers AND non-multiple of 3.
    c. Compressors hold columns
    d. 2 and 4 that are the least two even positive integers AND non-multiple of 3.

By following solution in point number 3 and 4, the following matrixes is generated to represent plan 1 and plant 2 respectively:

Matrix Representation of Plant 1 process flow diagram						
		1	2	3	4	5
		(Distillation 1)	(Compressor 1)	(Reactor 1)	(Compressor 2)	(Distillation 2)
1	A					
2	B					
3	X					
4	M					
5	N					
6	Y					
7	G					
8	H					

Figure III-5: Matrix Representation of Plant 1, Hypothetical Example 2

Matrix Representation of Plant 2 process flow diagram							
		1	2	3	4	5	6
		(Distillation 1)	(Compressor 1)	(Reactor 1)	(Compressor 2)	(Distillation 2)	(Reactor 6)
1	A						
2	B						
3	X						
4	M						
5	N						
6	Y						
7	G						
8	H						

Figure III-6: Matrix Representation of Plant 2, Hypothetical Example 2

By this end, the representation phase is accomplished. One essential aspect is held for the coming section is the numerical fill of the matrixes shown above. This is referred to as encoding. The process flow diagrams that are represented in the matrix should be fully encoded. The encoding specifications depends on the type of the encoded equipment and what is to be found from the particular element. In other words, the encoded matrix can simply indicate or defined the function of a given equipment. The rules and generation of encoding guides to these matrixes are represented in Systematic Procedure Input Advanced Stage. It is kept separate to the primary level

input section since the encoding require precise information about the output to be designed accordingly. The encoding input information are to be addressed.

III.1.4 Conclusions

In this sub-section, the primary level of data input synthesis towards systematic procedure are formulated and represented. In the formulation phase, the important parameters to defined a give system (plant) are identified. Then these parameters are classified into sets based on category. After categorizing the data, the representation phase considered gathering this information into one useful framework required for later data extraction and data access. In the representation phase, a matrix form is used to represent the framework of the categorized parameters identified earlier. An advanced data input setup is available in the coming sections to address the encoding of the flowsheet (fill up the matrix with numerical values). Briefly, this subsection provide the general specification of data input required to systematic procedure synthesis towards structural integration.

III.2 SYSTEMATIC PROCEDURE OUTPUT

The output of the systematic approach towards structural integration is simply the integration opportunities. In this section clarification about the input manner is made clear. Indeed, the developed approach is claimed to provide the user with additional factors to be considered for decision-making during the design activity. In the context of this work, these factors are defined as the synergetic opportunities. Hereby, a disclaimer is stated clear that the systematic approach provides opportunities towards integrated design but not design recommendations. Additional to this, it is worth mentioning that the developed approach does not guarantee benefits when its outputs are applied. More precisely, the application of the identified opportunities may or may not result in benefits. The benefits outcomes depend on many factors other than the initial idea or opportunity gate that is identified by the approach. These factors are many, for example but not limited to, the initial selection of the plant, the accuracy of the data input to the algorithm flowchart, the implemented design out of the algorithm, the accuracy for the implementation the later, the experience of the design engineer in the field of process design and probably simulation. These points/disclaimers are made clear for the purpose to properly provide the correct path towards development of this principle for future work as well as to provide the right understanding of the power/benefits that can be obtained from the developed approach for best results output.

The areas of process engineering research and development are related back to the seven themes/directions identified earlier. Hence, synergies are found accordingly. By understanding the significance and impact on every operating unit, and process design and synthesis under consideration of the seven themes, synergies can be identified. tool

The synergy types are directly related to the equipment types and possible savings. Since the purpose of this research is the core of the process (the reactors and the separation), the reactor

systems and separation systems are identified for algorithm flowcharts generation. Before moving to specific aspects of synergy types outputs, the general routes of synergetic opportunities are identified and classified. In order to identify the possible routes, generally, of the algorithms, the following routs are identified that hold for all synergy types:

1. Direct Share of Tasks
    a. Identified by identical chemical species flow around a give task
    b. Chemical specie attribution should be specified.
    c. No composition specification
    d. No operating condition specifications

2. Indirect share of Tasks
    a. Sharing a task require altering the design
    b. Identified by available Chemical Species Flow Around a give task
    c. Has constraint based on component attribution and relative property
    d. Constraints on source and final destination of a task
3. Dual Opposite Task Elimination

    This is a general type for many specific examples that may take place in a chemical plant. In general, performing a task is associated with capital, operating and utility cost, and sometimes, raw material, and thus avoiding performing it is a desired option, keeping the objective of excusing the task satisfied. This may be possible in case there is an opposite task that has the reverse objective. Thus, this type is dedicated to sort out the opposite tasks to ultimately eliminate them while maintaining their objectives. Briefly, the following hold:

a. Reverse a task to satisfy a forward need of another task

b. Constraints on the source and final destination of the task

4. Alteration of a Task

a. Common tasks executed differently

b. Constraints on source and final destination

Every algorithm flowchart follows the formulation represented earlier. In this section two main algorithms are presented, namely reactors and separation algorithms with their respective set of rules.

An important disclaimer needs to be stated here: this research does not claim that the identified synergy types nor specific routs fully describe all possible opportunities that maybe used nor completely utilizes the synergies identified via the later developed method

III.3 SYSTEMATIC PROCEDURE INPUT: SECONDARY SPECIFICATIONS

To make the algorithm flowchart searchable in, for example a computational program, the input information which are the sets that are translated into matrixes need to include numerical representation within the respective matrix, or simply encoded. As illustrated earlier, the input information such as processes, operating units, and chemical species are translated into numerical values and arranged into a matrix. Hence, the algorithm flowchart searches across the first second and/or third dimensions of a generated three-dimensional matrix while conducing decision/steps/actions based on the encoded system by numerical input. The arrangement of the elements is instructive. The encoded numerical input in the matrix follow particular roles to systematically address and eventually approach the system of interest. The general approach for generating an algorithm flowchart for a given synergy type is as per t the following:

1. Sets involve numerical values
2. Every dimension of the three matrix dimension represents a set. Specify the set of unit operation types involved. For example: reactors, separators, etc.
3. Provide every type of unit operation with a unique set of numbers. For example: odd, even, prime, multiple of a number etc.
4. The used dimensions are Z elements represent the involved processes or plants (can be noted as P set), Y elements represent involved unit operations/equipment in all participating plants (set E), and X elements represent all chemical components types under given synergy type (set C).
5. Y elements (equipment and unit operations) are generated as per to the involved can be easily modified for development purposes or adjustment purposes

Table III-1: General Set of Rules for Encoding Unit Operation

Unit Operation	Separators	Reactors	Combination Units
Coefficient Magnitude	Driving force Example: relative volatility, relative molecular size OR Role in Mixture	Attribution	Role in a mixture, 1-pure, 2 binary, 3 ternary etc.
Coefficient Sign	Category of components for relative driving force Example Solute/solvent Heavy key/light key	Category of components whether it is Predicted Consumed	Category Purchased as raw material Produced/recovered in the process

6. In case of existence of multiple classes of any equipment category identified above, the magnitude digit can be adjusted, for example, 10s for first class, 20s for second and so forth.
7. Search among the matrix takes into consideration identification of common chemical species
8. instructions are built-up to identify the opportunities of different routes that are in the level of the general chemical system.
9. These routs can be found in one or more synergy type.

10. One synergy type can have one or more route

11. Routs are identified by verifying the seven themes of process engineering research

These rules and instructions are used for the implementation of the specific algorithm flowcharts in this research. These impetrations are specified in details in the following sections.

III.4 SYSTEMATIC APPROACH IMPLEMENTATION (TRANSFORMATION FROM INPUT TO OUTPUT)

III.4.1 Introduction

The transformation of the input to the output is performed by sequential execution of steps. In the context of this work, knowledge about the input and the output is essential for the design of the of the steps. This sequential execution of steps can be represented by a flowchart of an algorithm. These algorithm flowcharts are designed based on every desired output. The main two requirements of the algorithm flowcharts are data processing that is defined as the obtainability of data of meaning via a collaborative execution of data representative [18] and automated reasoning. Also, the algorithm address simple intermediate calculations throughout number of implemented loops.

The algorithm flowchart framework is implemented in this research because of its multiple benefits. Basically, an algorithm can be defined as an untimely workable method of a specified problem that provides expression of full set of instances [19]. Because in this research, an operating unit can be appreciated form multiple perspectives to properly integrate it in terms of its structure, it is beneficial to employ a method that allows searching across multiple instances or what is donated to in this framework as routes. In this section, navigation through the data input that is design as per to other needed output is conducted in order to generate the outputs towards the algorithm.

III.4.2 Separation

III.4.2.1 Description

. The systematic approach is implemented to involve separation systems, specifically distillation columns, towards structural integration. In general, separation systems acquire vital

place in chemical processes as their function majorly contributes in defining the core structure of many chemical processes. Distillation columns represent one separation technique that is frequently used in chemical processes. Basically, separation by distillation works on the principle of the simple alembic that separates homogenous mixtures which their components have difference in relative volatility. Thus, the driving force towards this separation technique is relative volatility. As equipment, distillation by separation in chemical processes is operated in columns. Thus, a distillation column consists of a tower that is attached by a reboiler and a condenser of which the later acquires a reflux drum and a pump in most cases. Despite industrial and technical importance of distillation columns, they are energy intensive. Not only energy intensive, but also, their capital cost is frequently observed to acquire a good percentage amount of the total; plant capital cost. These two factors make distillation columns an interesting case to be addressed in structural integration.

An algorithm flowchart is dedicated to address distillation columns. This algorithm flowchart aims to search among separation units for a given process to identify possible synergetic opportunities. The assumptions that to be considered in this while appreciating the separation algorithm flowchart are as follows:

1. Only distillation columns are the systems that are applicable for the usage
2. Always assume relative volatility is the driving force towards separations
3. Separations take place in a binary setup
4. Azeotrope distillations are excluded, yet they can still be encoded to search possible options.

5. Petroleum based components (i.e. wide range of hydrocarbon mixtures) can be used, however, the flowchart is not designed with a dedicated consideration to them.

This flowchart requires input specifications and provide particular outputs. Thus, the following two sections address these two parameters in sufficient details.

III.4.2.2 Input Specifications

The algorithm of Separation takes into consideration the following set of rules for encoding:

- Negative sign refers to components of light cut
- Positive signs refer to components of heavy cut
- Magnitude of a unity refer to the key component

One important comment for consideration is related to the extent of separation, in other words, how sharp the assumed separation is. In general, this is not considered, however, if there is a significant portion is distributed in each of heavy and light cuts for a given component, i.e. from 30 to 70wt% distribute on among cuts, the system of interest considers them as components that are formally distributed among cuts, and they have special input specification.

Table III-2: Encoding specifications input for Reactor algorithm flowcharts

Sign	Implication	Magnitude	Implication
Negative	Components of light cut	1	Light Key Component
		2 to infinity	Light Non-key component with direct proportion with deviation in boiling point from the light key component
Positive	Components of heavy cut	1	Heavy Key Component
		2 to infinity	Heavy Non-key component with direct proportion with deviation in boiling point from the heavy key component
	Distributed between light and heavy cuts	12	Tends more towards the light cut
		21	Tends more towards the heavy cut

III.4.2.3 Output specifications

The overall aim is to be able to structurally integrate distillation columns across plants. By moving to a deeper objective, the distillation columns source of deficiency is highlighted to properly hit the previously stated targets. The capital investment on distillation column is believed to have a reduction opportunity if columns of similar tasks are merge with a disclaimer that this opportunity does not necessarily promise savings. As per to operating cost, it is expected to be affected indirectly by the complete/partial share of tasks. Thus, the following synergetic opportunities may be obtained from the algorithm flowchart of separation:

1. Direct-common separation tasks
2. Same separation task after altering separation sequence.

In the context of this work, a separation task is defined as subjecting a mixture of fluids that essentially contain components of minimum number of 2 to separation of where the separation results in at least n-1 separated mixtures/pure components contained I the original mixture, where n is the number of components originally exist in a mixture.

III.4.2.4 Algorithm Flowchart

An algorithm flowchart is implemented in this section to properly fit the defined input and output specified earlier. The flowchart is written as per to the encoded input, and hence a translation between the encoded flowsheet and the original process flow diagram is provided in a table. The algorithm problem is to figure out the needed output from the given input defined earlier, and accordingly it is implemented. The flowchart of the algorithm is illustrated in Figure III-7 This algorithm flowchart considers instructions as per to the encoded input, and subsequently the instructions are encoded. Thus, Table A-2 in Appendix A is written to provide the necessarily

understating to the developed flowchart. It is divided into four main sections that are the number of the block in the flowchart, the role of the block, whether it is being intended for decision making, stating an output etc., the original statement presents in the flowchart, and the practical implication towards the given instruction.

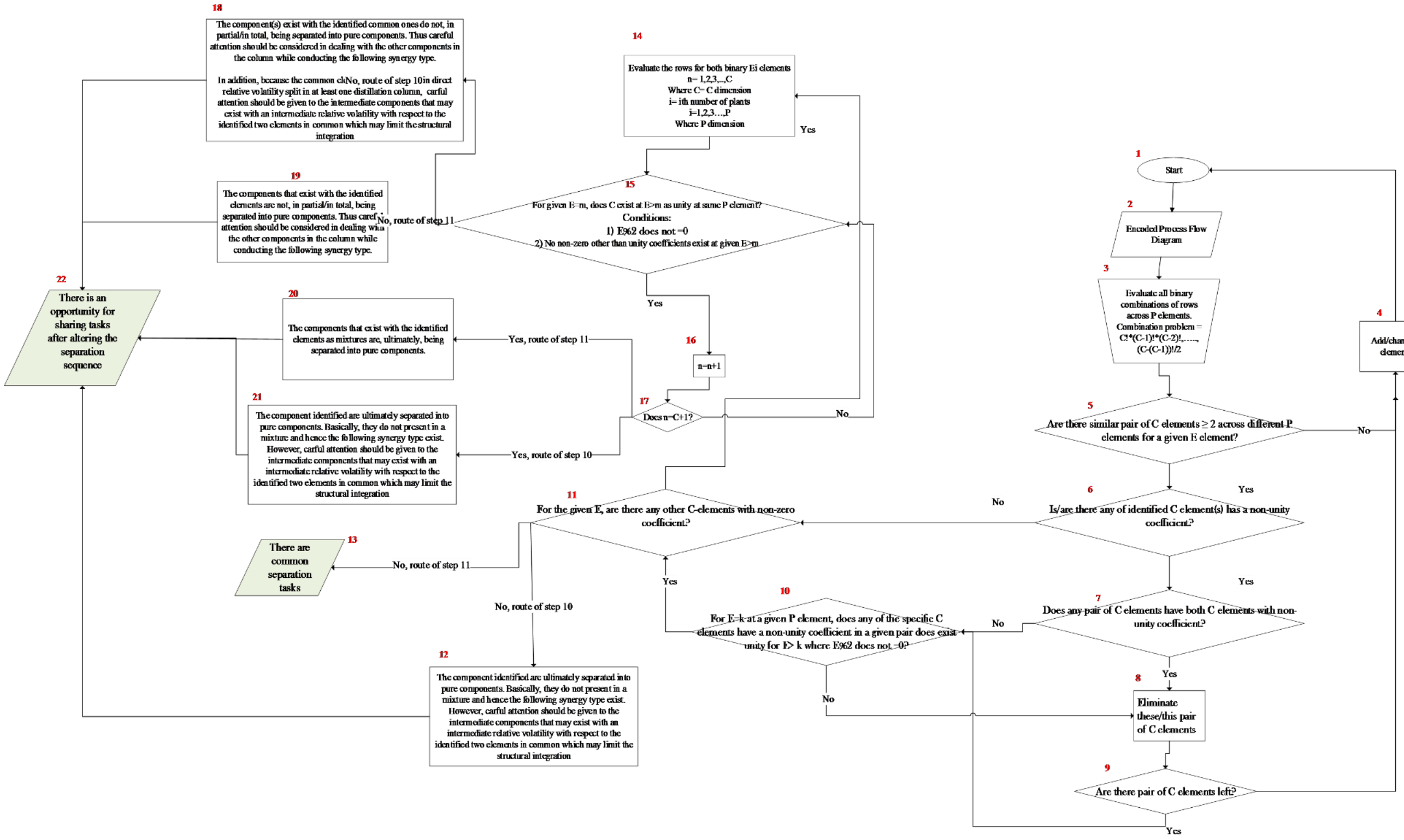


Figure III-7: Algorithm Flowchart Towards Structural Integration of Separation

Hypothetical Example 3: implicit common separation task

In this example, there are two plants as shown in Figure III-8, specifically, a separation section of each plant are subjected to structural integration algorithm flowchart. In plant 1, a feed of four components mixture is being separated in pure components streams. In Plant 2, a ternary feed mixture is being separated into pure component streams. As it may be observed that there are two components in common among the two plants, namely, B and C. The problem that there might be not a direct task share because the original combination of the distillation columns sequence arrangement of the two plants does not allow direct share of tasks. These two plants are subjected to structural integration algorithm flowchart to identify whether there is a possibility to structurally integrate the separation sections of interest.

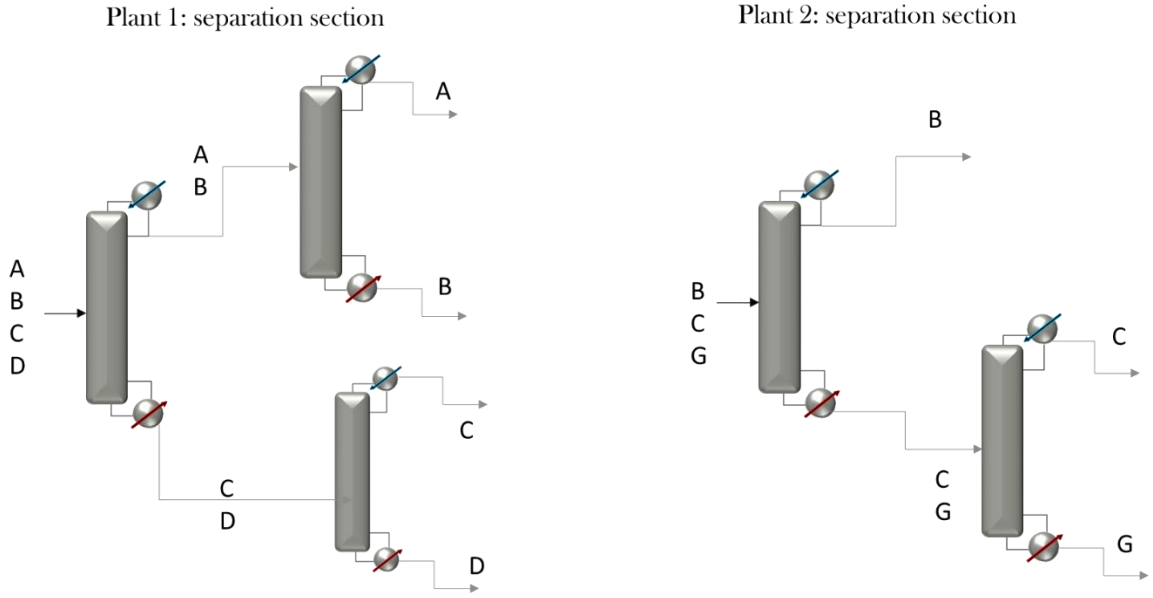


Figure III-8: Schematic diagram of plants discussed in Hypothetical Example 3

Solution

As shown in Figure III-9, in the first step, by passing through the manual loop of step number 3, when verifying the binary combinations of rows, two common elements (C elements) are found across plants (P elements) for a given distillation column (E element) per plant (per P element). Specifically, these are elements B and C. Then, by passing through step 6 and 7 to eventually conclude that all elements are actually key components (all carry unity coefficients), it goes through step 11. In step 11, the system should identify that the other components in the columns of interest (where the common C elements are found) has non-key components (carry coefficients of non-zero). These elements are highlighted in the matrix of the same figure. Then, when it passes through the loop that starts with step 14, it eventually detects that all of those elements that are found in the same column as non-keys, are also found as key-component elements in later columns (meaning that they are being separated to pure components). Thus, the synergy that is identified: The components that exist with the identified elements as mixtures are, ultimately, being separated into pure components and hence Synergy of common separation tasks is available after altering the separation sequence.

steps: 1,2,3,4,6

Plant 1

	1	2	3	4	5
A=1	-2	-	-1	-	0
B=2	-1	-	1	-	0
C=3	1	-	0	-	-1
D=4	2	-	0	-	1
G=5	0	-	0	-	0

Plant 1

	1	2	3
A=1	0	-	0
B=2	-1	-	0
C=3	1	-	-1
D=4	0	-	0
G=5	2	-	1

steps: 11

Plant 1

	1	2	3	4	5
A=1	**-2**	-	-1	-	0
B=2	-1	-	1	-	0
C=3	1	-	0	-	-1
D=4	**2**	-	0	-	1
G=5	**0**	-	0	-	0

Plant 1

	1	2	3
A=1	**0**	-	0
B=2	-1	-	0
C=3	1	-	-1
D=4	**0**	-	0
G=5	**2**	-	1

steps: 14,15,16,17, and ends with 20 with identitfed synergy

Plant 1

	1	2	3	4	5
A=1	**-2**	-	**-1**	-	0
B=2	-1	-	1	-	0
C=3	1	-	0	-	-1
D=4	**2**	-	0	-	**1**
G=5	**0**	-	0	-	0

Plant 1

	1	2	3
A=1	**0**	-	0
B=2	-1	-	0
C=3	1	-	-1
D=4	**0**	-	0
G=5	**2**	-	**1**

Figure III-9: Encoded Matrix of hypothetical Example 3

III.4.2.5 Summary

In this section, the implementation of the systematic approach developed subjected separation system of distillation columns category. The main motivation towards the selection of this category is its frequently noticed high capital and operating costs. The problem is defined as figuring out synergetic opportunities towards structural integration of distillation columns across process boundaries. Identified general opportunities are direct and indirect share of separation tasks to eventually represents the final destination of the developed flowchart. The input specification requirements are represented by the developed approach earlier, namely the encoded flow diagram that is represented by 3 dimensional matric, enclosing sets of plants, equipment, and components. The method towards transforming the input to the output specified is represented by

an algorithm flowchart. The algorithm flowchart is explained by translating the instruction that re built on the bases of the encoded input into practical implications. Then, a hypothetical example is conducted in order to provide an idea about how does the developed method work, illustrating one route. Briefly, this section contains the implementation of the developed systematic approach, subjecting the separation systems of distillation columns type towards structural integration across plants boundaries.

III.4.3 Reactors

III.4.3.1 Description

One implementation of the systematic approach subjects the reactors. Reactors algorithm flowchart is implemented to identify synergies for integration opportunities by searching among reaction systems. Reactors are the heart of the chemical processes. The essence of considering reactors for structural integration can be represented by highlighting their importance in the context of chemical processes. The performance of the reactors has a significant effect on the subsequent steps in the process. This can simply be evident by looking back into the Onion diagram presented in earlier sections. The separation and recycle layer comes after defining the reactor layer. In terms of technical reasoning, the production quality and possibly capacity of a particular reactor determines the separation type, size etc. as well as the recycle systems. Indeed, one of the main objectives of recycle system is to recycle the unreacted material in the reactor. The unreacted material results from incomplete conversion of reactants, bringing the argument back to the reactor systems. These facts make the reactors subject of interest for process performance enhancement attempts. In brief, implementation of reactor systematic approach requires a clear input and a clear output, and a clear implementation in terms of the steps being designed and selected choices.

III.4.3.2 Input Specifications

To involve reactors in structural integration, its input parameters need to be identified, analyzed and classified in order to properly manipulate the reactors into the structural integration opportunities. Reactants and products represent the main elements in a reactor, then the catalyst, operating conditions etc., may serve as reactor parameters. Because the catalyst, temperature, pressure, size etc. of a given reactor are mostly fixed based on the desired production, they are considered as secondary parameters, at least within the context of this work. Furthermore, because as stated earlier, the established structural integration is expected to mostly result in re-implementation of the plants, the identified synergy types are set accordingly. The main parameters, and the most basic ones, namely reactants and products are subjected to analysis. These parameters are sufficient to describe the flow of chemical species around a given reactor. By looking into these parameters deeply, it can be found that they are classified into categories within their primary categories. Precisely, the products in every chemical system are classified as per to the context of the process. These classifications may be main products, by-product/side products, co-products, waste, etc. This also applies to the reactants. The reactants can be classified into categories as per to their consumption rate for either being fed in excess, at the stoichiometric ratio, or as limiting reactants. Another classification of reactants can be considered is the source. One source category maybe a fresh feed, that is a raw material, while the other one maybe a utilized product/unreacted material in the process itself. These considerations briefly address the parameters that are taken into account while conducting the overall reasoning of the reactor systems. The attributes of every chemical specie available in the system of interest is distinguished by the different encoding parameters. These parameters can be classified as per to the set of rules shown earlier. Hereby, the following set of rules give brief picture about system:

6. Sign: determines production or consumption
7. Magnitude: determines attribution

Table III-3: Encoding specification input for reactor algorithm flowchart towards structural integration

Sign	Implication	Magnitude	Implication
Negative	Chemical specie is being consumed (reactant)	1	Limiting reactant-fresh feed
		2	Fed in excess-fresh feed
		range 5 to infinity	Intermediate process feed
Positive	Chemical specie is being generated (produced)	1	Main Process Product
		2	Main Reactor Product
		3	Co-product
		4	Legal/direct waste
		range 5 to infinity	Side products

III.4.3.3 Output Specifications

Another factor that plays an essential role in involving the reactors in structural integration is the final destination of the designed approach. The destination of the systematic approach that considers reactors is simply the output. As addressed earlier in this work, there are number of synergetic opportunities that may be obtained by looking into the chemical systems in general.

These general opportunities are used to represent the more specific cases to fit the context of chemical reactors. In reactors, it is can be observed that some reactors may have the same feedstock in partial or in total, which applies similarly to the products. Also, some reactors may be identical in terms of the flow of chemical species regardless and with regard to the selectivity's. Furthermore, some reactant may share part of the feed with all products and vice versa. These reasoning about the reactor systems led to the identification of several synergy types.

III.4.3.4 Algorithm Flowchart

The input and output requirements specified earlier in this section with specific consideration of reactor systems are gathered in one full representation of the system to untimely have one representation via an implemented approach towards structurally integrating reactors. The implementation is designed in order to obtain the needed output from the given inputs. This Flowchart is shown in Figures III-10 through III-13. Additional to that, as per to the representation in the separation section, the flowchart that is mostly encoded is translated back into a practical implementation in Appendix A. The reactor algorithm flowchart is subjected to fragmenting in order to enhance the visualization of the text. The figures that follow the overall flowchart are parts of the flowchart.

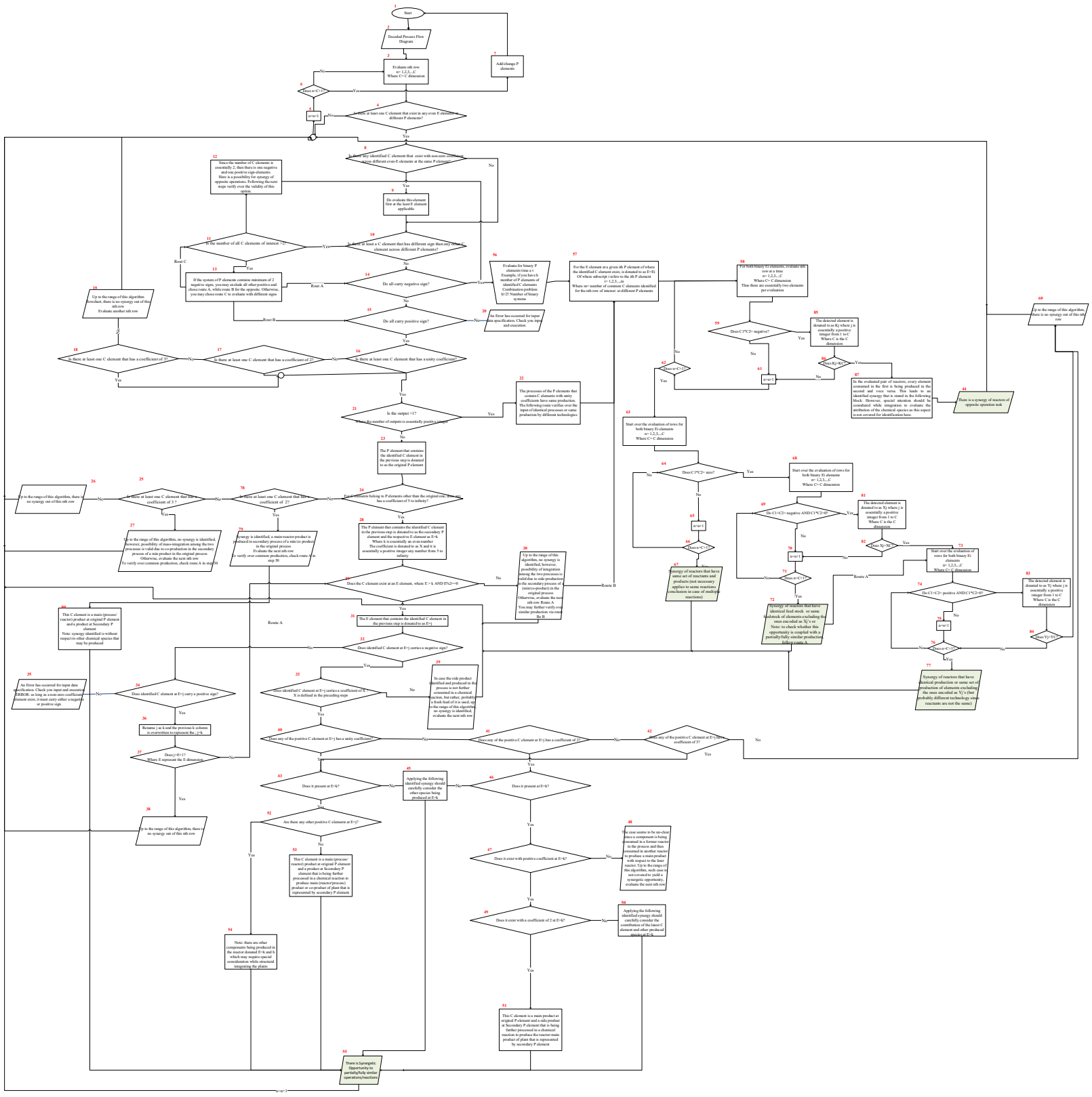


Figure III-10: Algorithm Flowchart Towards Structural Integration of Reactors

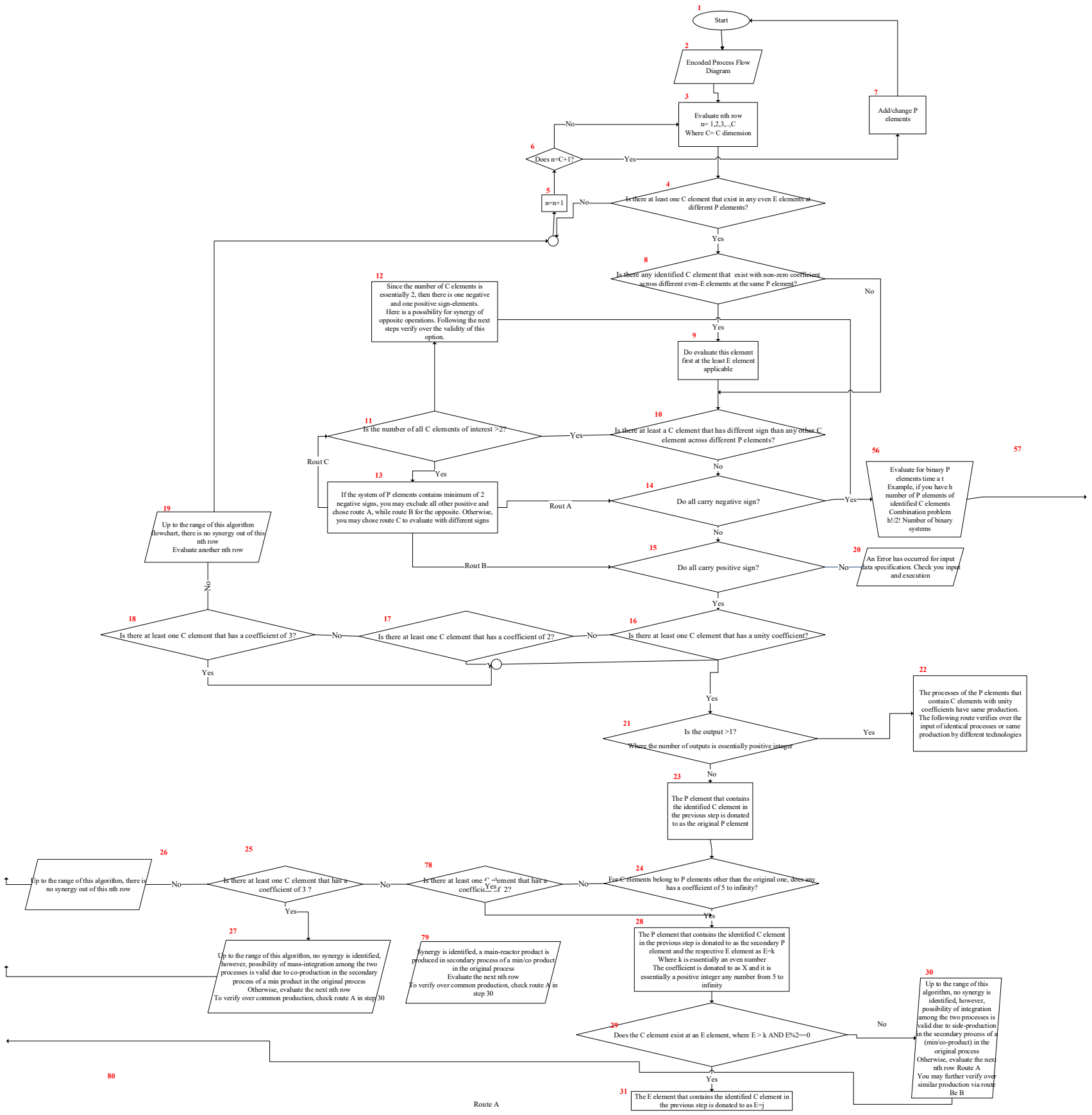


Figure III-11: Part A of cropped reactor Algorithm flowchart (for visualization)

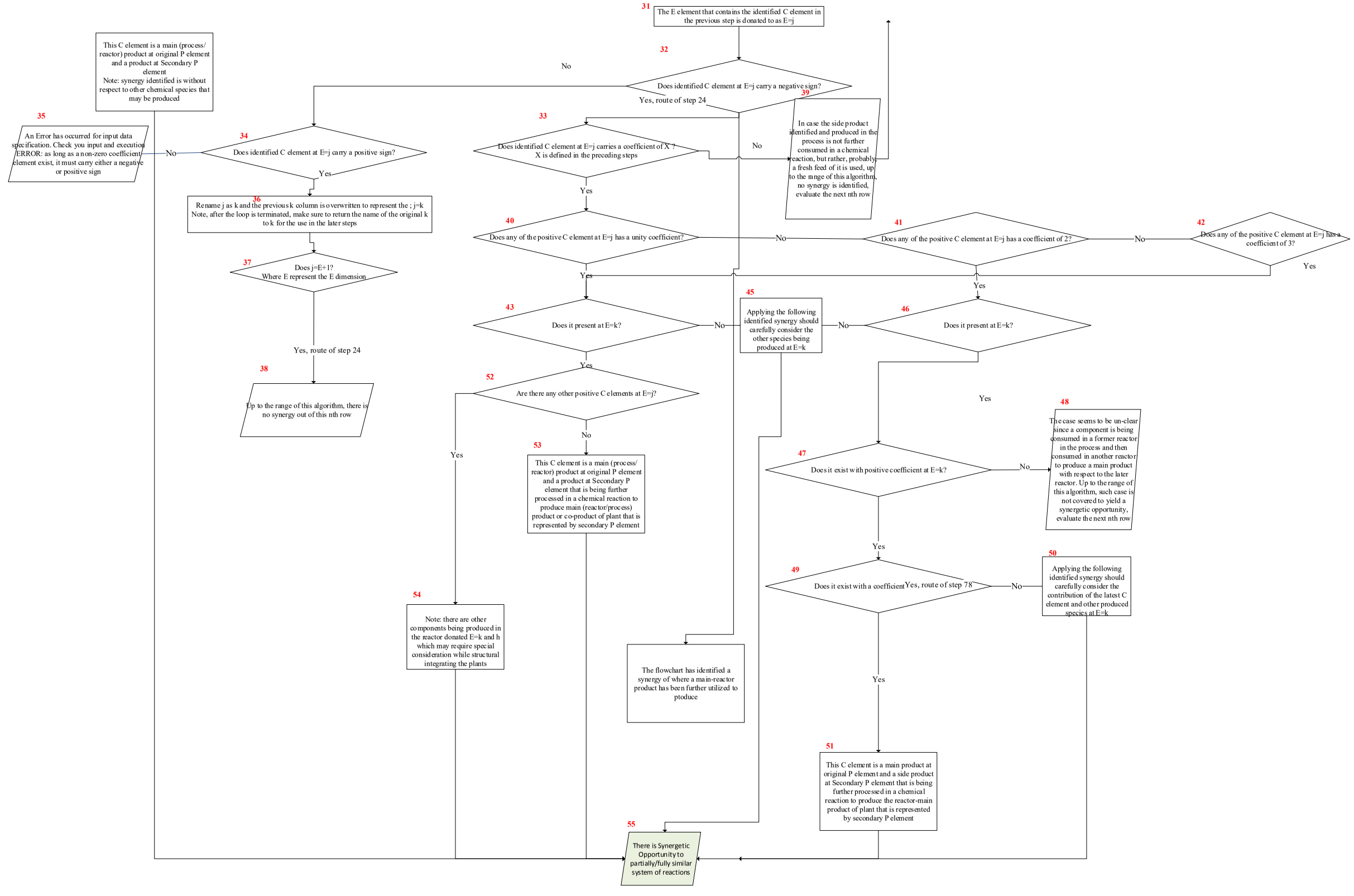


Figure III-12: part B of cropped reactor Algorithm flowchart (for visualization)

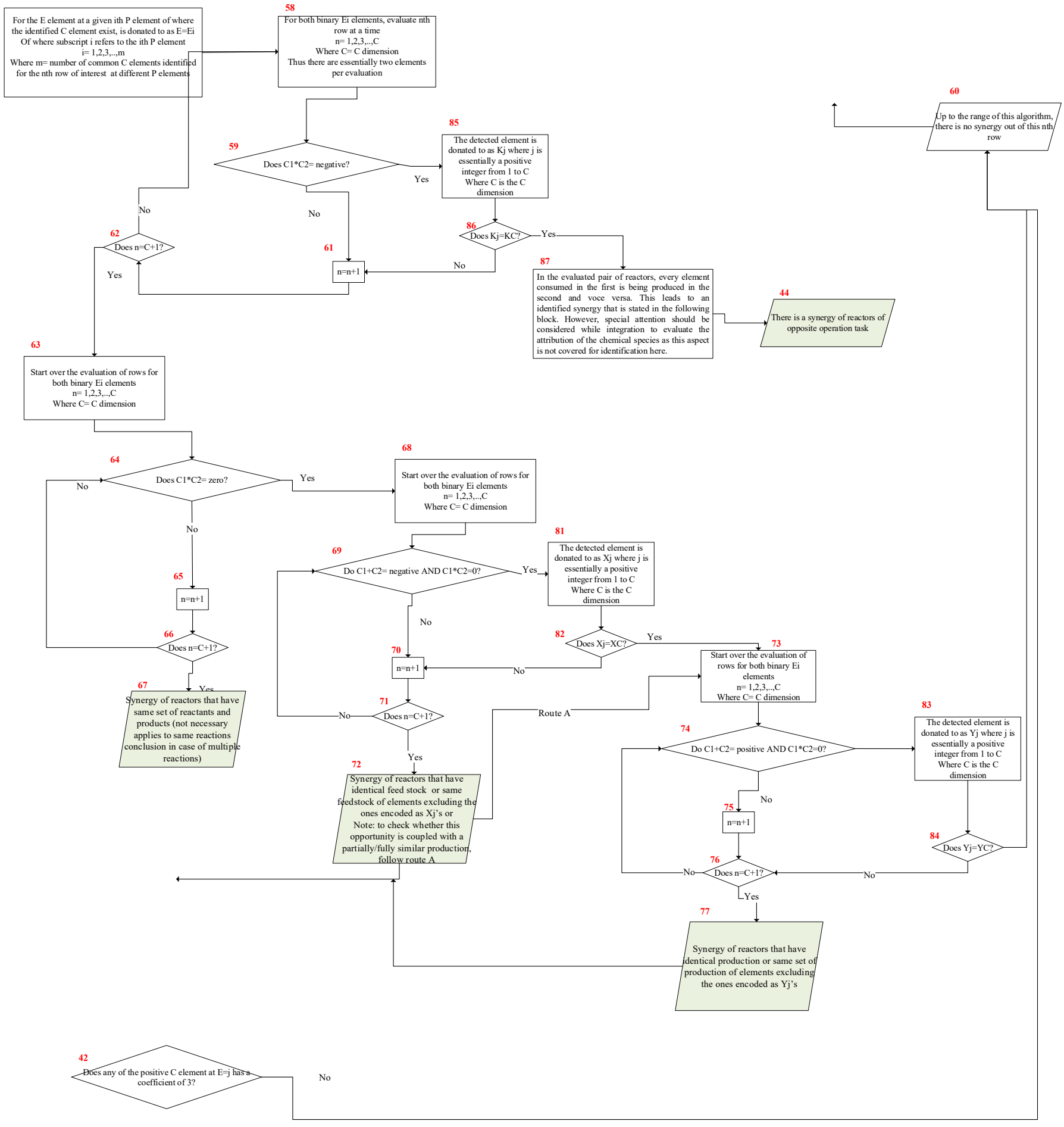


Figure III-13: part C of cropped reactor Algorithm flowchart (for visualization)

Notes on the Numbers of the blocks:

a. The numbering is not followed with exact respect to the existence of the blocks in the flowchart because many blocks have multiple outputs as well as inputs which makes ordering not straightforward.
b. Some blocks numbers widely deviate from the contexts of numbers of the neighbors blocks. The reason behind this that the addition of blocks and modifications took place after the original numbering was fixed. Thus, the numbering does not influence appreciating of the blocks, it is used just to provide a code/number reference to the flowchart.

Hypothetical Examples

Hypothetical Example 4:

As shown in Figure III-14, In plant 1, component M is a main product, and F is a side product. In plant 2, with different reactant, component H is a main product, and M is a side product. In reactor 2 of plant 2, M is being further utilized as a reactant to product H (main product), and K as a side product.

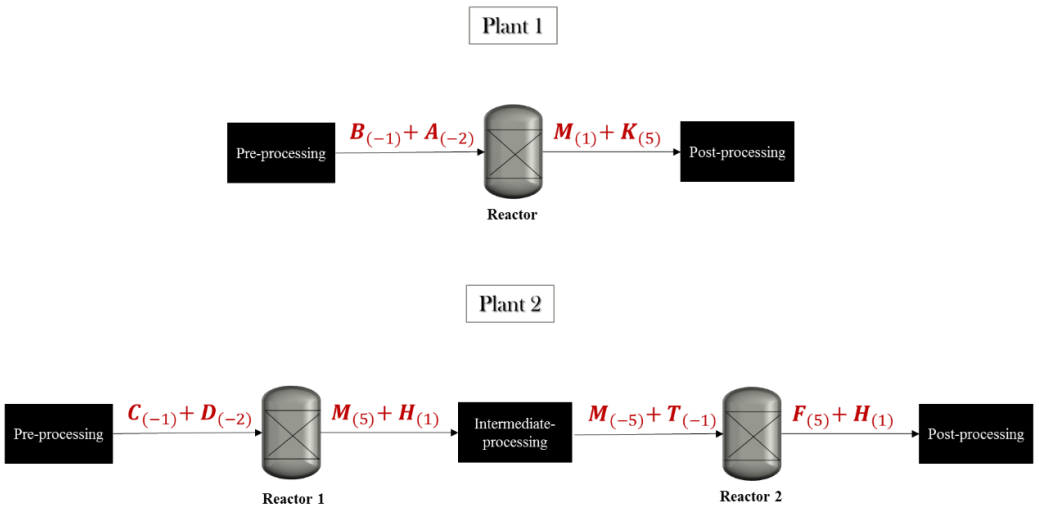


Figure III-14: Schematic Drawing of plants in Example 4

Solution

As shown in the Figure III-15, by the start of the flowchart, rows 1 and 2 are by-passed because they contain common elements, while a common element could be detected at row 3 and hence evaluation is made based on row 3. It then follows the flowchart through steps 10, 14, 15, 16, 21, 23, and 24 to eventually donate Plant 1 to an original P element while Plant 2 to a secondary P element which are the nicknames of the plants in order to proceed with the flowchart accordingly. By here, the flowchart detected that the identified column element represents a main product with respect to process 1, and a side product in the one reactor in plant 2. Then, via steps 29,31,32, and 33 it shows that could detect consumption of the produced side product of Plant 2 in a later reactor in the plant. Then, questions about other elements in the later reactor are conducted just to identify the significance of the consumption of the side product that has been utilized to whether produce a main product, legal waste, etc. Then by step 55, it shows that this setup leads to the synergy of partial total removal of reactors.

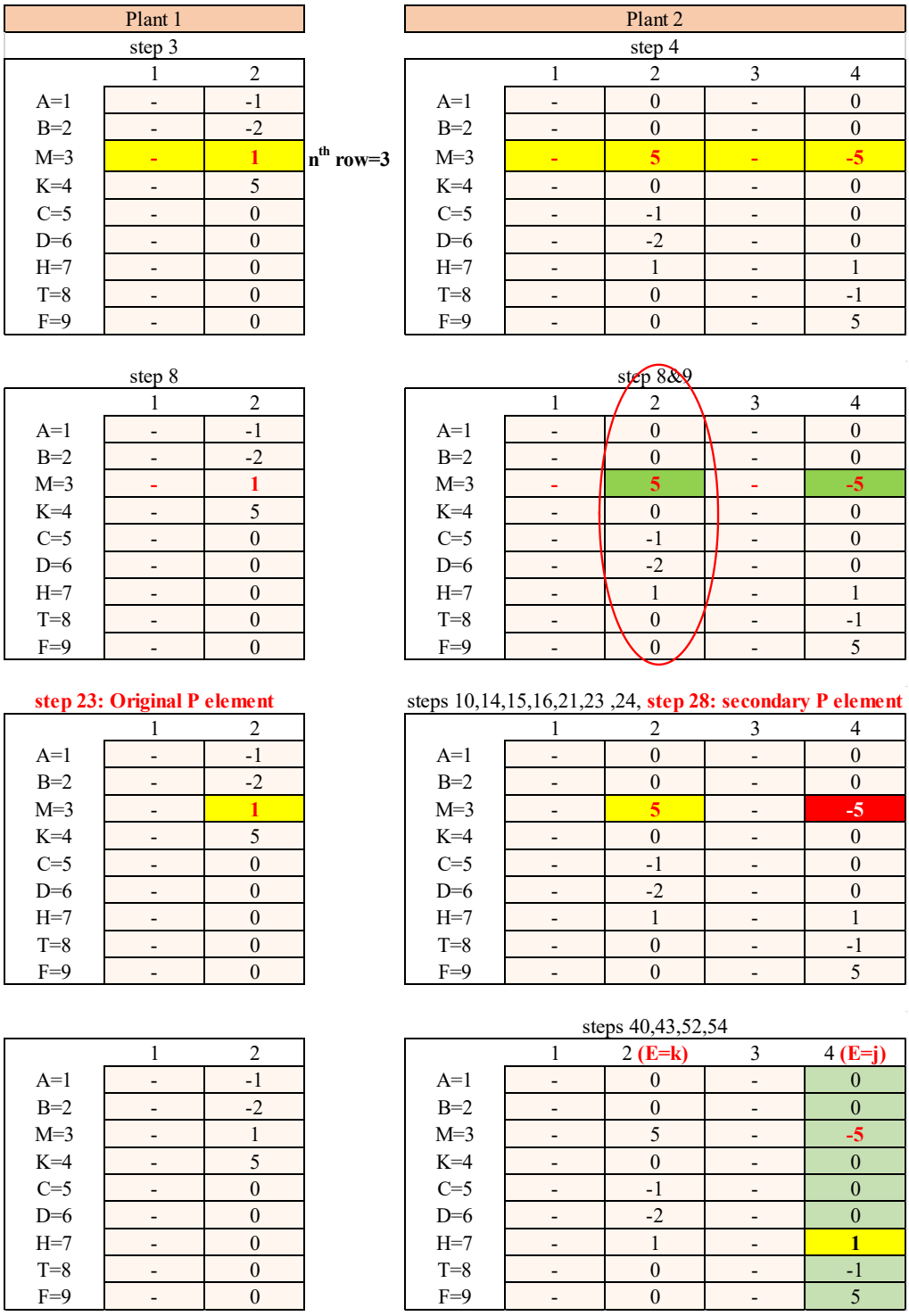


Figure III-15: Encoded Matrix of synergy identification, Hypothetical Example 4

Hypothetical Example 5: Same Feedstock

As shown in Figure III-16, In this example, two plants are subjected to structural integration. The reactors flows (reactions per reactor) of each plant are shown in the figure. In plant 1, C is produced as a main process product, while D as a side product by consuming component B and A of which the latter is fed as the limiting reactant. In plant 2, there are two reactors, reactor 1 produces B as the main process product by consuming F and M of where the former is fed as the limiting reactant. In the second reactor, C is produced as a reactor-main product with G as a side product by consuming A and B of where the former is fed as the limiting reactant.

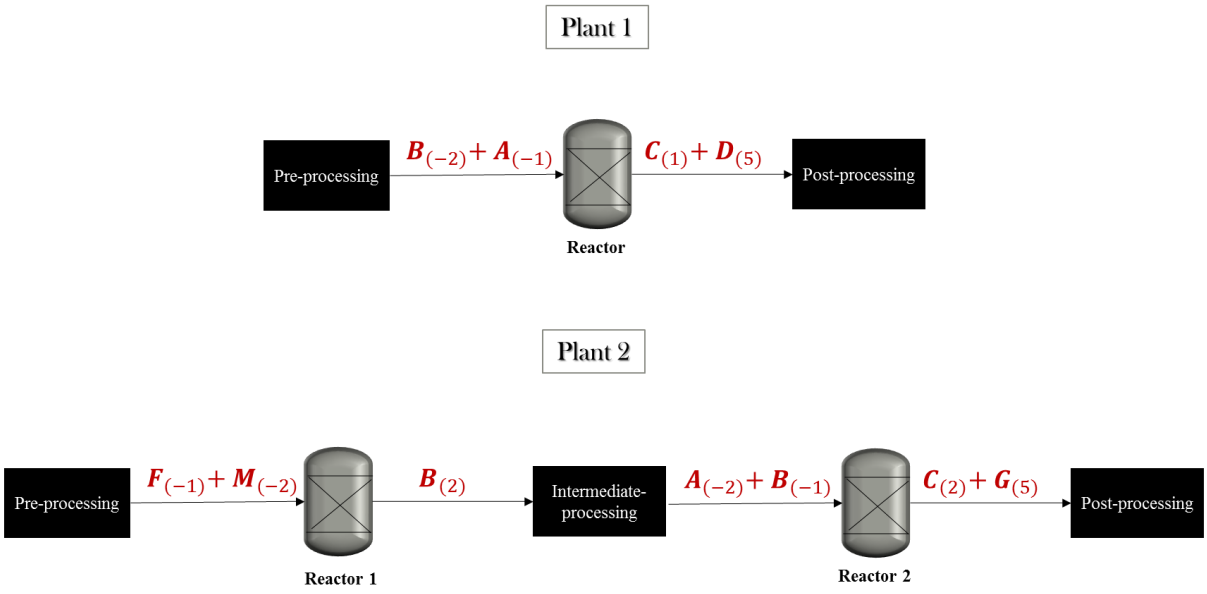


Figure III-16: Schematic diagram of systems discussed in Hypothetical Example 5

Solution Part 1:

As shown in Figure III-17, step 59: none of C components of the highlighted columns give result in negative value by multiplication, thus, loop passes to step 63 after checking all rows Step 63: As highlighted in yellow in the matrix, the multiplication results in a zero, hence the loop is bypassed to step 68 once this condition is satisfied. Loop starts with step 68: the loop checks over all C components row by row across the highlighted columns until it detects two elements that their summation is negative while their multiplication is 0. Since this condition is not valid to any, the loop is by-passed to output 72. Output 72 shows that there is a common feedstock as a synergy among the two plants. Then it by-passed to via route A to check over the production, to eventually detect that there is one element in common among the products while two are not in common. Hence partially common production. Note, in case of existence of a third P element (third plant) the flowchart should go back to the manual loop of step 56 to validate it in the context of all possible binary combinations of P-elements available

Plant 1			
	1	2	
A=1	-	-1	n^{th} row=1
B=2	-	-2	
C=3	-	1	
D=4	-	5	
F=5	-	0	
M=6	-	0	
G=7	-	0	

Plant 2				
	1	2	3	4
A=1	-	0	-	-2
B=2	-	2	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Steps 9, 10, 14, 56, 57, 63 by-pass to 68

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	0	-	-2
B=2	-	2	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Step 68 ito 72 output: identical feedstock

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	0	-	-2
B=2	-	2	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

By-passed to 73 via Route A: synergy of partially common production

	1	2	
A=1	-	-1	
B=2	-	-2	
C=3	-	1	
D=4	-	5	Y1
F=5	-	0	
M=6	-	0	
G=7	-	0	Y2

	1	2	3	4
A=1	-	0	-	-2
B=2	-	2	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Figure III-17: Encoded Matrix and illustration towards synergy identification of Hypothetical Example 5, part 1

Solution part 2:

As shown in Figure III-18, After evaluating the first row detected of similar elements and giving an output synergy, the algorithm flowchart returns the system back to the initial loop that checked over the rows available. Since the next row, that is of n=2 does not equal to C+1, that is 7+1=8, the flowchart steps would still process.

In the second round, the loop detects a common element across plants at the second row, namely, component B. Note that this element exists in two columns (two reactors) in one P element (one plant) the element that exist at the least is being evaluated according to the flowchart instructions. Then, it processes it through steps 8,9,10,11, and then since the two elements one is being produced while the other consumed, of which the case that is not associated with a specific synergy type, it returns the process back to the initial loop to step 5

Plant 1		
	1	2
A=1	-	-1
B=2	-	**-2**
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

n^{th} row=2

Plant 2				
	1	2	3	4
A=1	-	0	-	-2
B=2	-	**2**	**-**	**-1**
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Steps 8,9,10,11,12 back to 5

	1	2
A=1	-	-1
B=2	-	**-2**
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	0	-	-2
B=2	-	**2**	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Figure III-18:Encoded Matrix and illustration towards synergy identification of Hypothetical Example 5, part 2

Solution part 3:

In the third round, the loop detects common elements at row 3, to go through steps 8,9,10,14,15,16,21,24,78,79, to ultimately identify synergy at step 80. It identifies synergy of a common element that is a main-process product in plant 1 while being a main-reactor product in plant 2. Also, it further suggests to evaluate it over the identical production via route A in step 30. The latter is not illustrated here since it will be illustrated in later examples.

Plant 1		
	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

n^{th} row=3

Plant 2				
	1	2	3	4
A=1	-	0	-	-2
B=2	-	2	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Original P element

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

Steps 8,9,10,14,15, 16,21, 24, 78, 79 , and 80

	1	2	3	4
A=1	-	0	-	-2
B=2	-	2	-	-1
M=3	-	0	-	2
K=4	-	0	-	0
C=5	-	-1	-	0
D=6	-	-2	-	0
H=7	-	0	-	5

Figure III-19: Encoded Matrix and illustration towards synergy identification of Hypothetical Example 5,part 3

Hypothetical Example 6: Identical production

In this example, as shown in Figure III-20, two plants are participating towards structural integration. In plant 1, C is produced as a main process product, while F is produced as a side product by the consumption of components A and B, of where the former if fed as the limiting reactant. In plant 2, there are two reactors, the first produces C as a main product of the process while G as a side product by the consumption of A and M of where A is the limiting reactant. In the second reactor of Plant 2, C is further produced (that is the main product) with a side production of F by reacting G and K. G is the produced side product in the former reactor in the plant, while K is the limiting reactant.

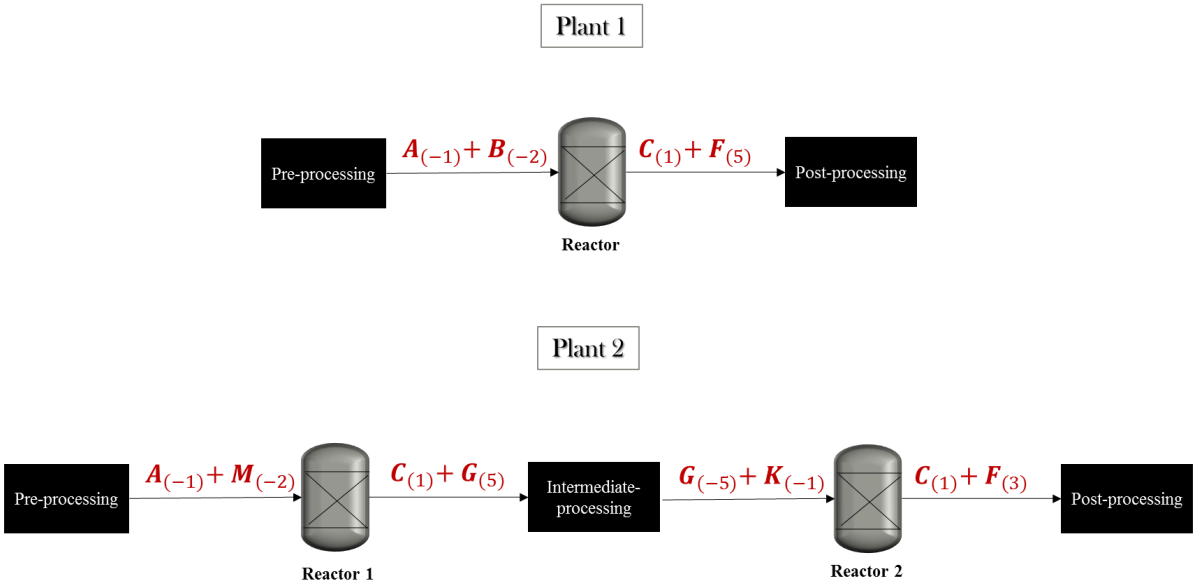


Figure III-20: Schematic diagram of systems discussed in Hypothetical Example 6

Solution

This case should result in synergy of identical production. Also, it should yield partially common reactants and products.

Solution part 1:

A shown in Figure III-21, once the encoded process flow diagram enters the algorithm flowsheet, it detects similar components across plants in the first row, and then moves to the following steps. Since all detected C elements are negative, it enters the first loop that starts by step 58 and by-pass it to loop 63 since no component across the reactors (columns) is being produced and consumed in the other reactor and vice versa. In loop of step 63, it detects two components of which each is consumed in one reactor while being absent in the other reactor, because there is a minimum number of common reactants, it gives the output of synergy of feed stock, and in this case, partially

similar feedstock. Then, the flowchart moves through route A to detect over the applicability of similar production, and similar to previous loop, it could detect two elements (products) that are not in common among the products, however, since there is a minimum number of one common product, it leads to the synergy of common product, and in this case, it is of the type partially common products excluding the detected ones that are not in common.

steps 8,9,10, 14,

Plant 1		
	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
F=4	-	5
M=5	-	0
K=6	-	0
G=7	-	0

n^{th} row=1

Plant 2				
	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
C=3	-	1	-	1
F=4	-	0	-	4
M=5	-	-2	-	0
K=6	-	0	-	-1
G=7	-	5	-	-5

Steps 56, 57, 58, 63, 64

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

Steps 68,69 to 72, partially common feedstock synergy

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

X1

X2

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

By pass through route A: Steps 73,74

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

Y1

Y2

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

step 77: synergy of partially common product

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

Figure III-21: Encoded Matrix and illustration towards synergy identification of Hypothetical Example 6, part 1

Solution part 2:

Reference Figure III-22. In the second round, row 3 is detected, it would pass through steps 8,9,10,14,15,16,21,22,57 since all detected species are with positive and further detected to acquire more than one component with a unity coefficient. Then it is bypassed to step 58, because there is no element across the plants its multiplication results in a negative sign (meaning that no element is actually being consumed in a plant while being produced in the other) the flowchart by passed it to the next loop that is 63. However, it detects two multiplications as zero for the negative, donating them as X1 and X2, while one common specie of summation of negative and multiplication results in a non-zero value, meaning that the component exists as a reactant in both plants' reactors. Then it is bypassed to check over the production, and as shown in the figure, it does detect one common and two not in common as products to give a synergy of similar production in this case for partially common production.

steps 8, 9, 10, 14, 15, 16, 21, 22, 57,

Plant 1			
	1	2	
A=1	-	-1	
B=2	-	-2	
C=3	-	1	n^{th} row=3
F=4	-	5	
M=5	-	0	
K=6	-	0	
G=7	-	0	

Plant 2				
	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
C=3	-	1	-	1
F=4	-	0	-	3
M=5	-	-2	-	0
K=6	-	0	-	-1
G=7	-	5	-	-5

Steps 58, 63

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

Steps of the loop that starts with 68 to 72: synergy of partially similar feedstock

	1	2	
A=1	-	-1	
B=2	-	-2	X1
C=3	-	1	
D=4	-	5	
F=5	-	0	X2
M=6	-	0	
G=7	-	0	

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

Steps of the loop that starts with 73 to 72: synergy of partially similar products

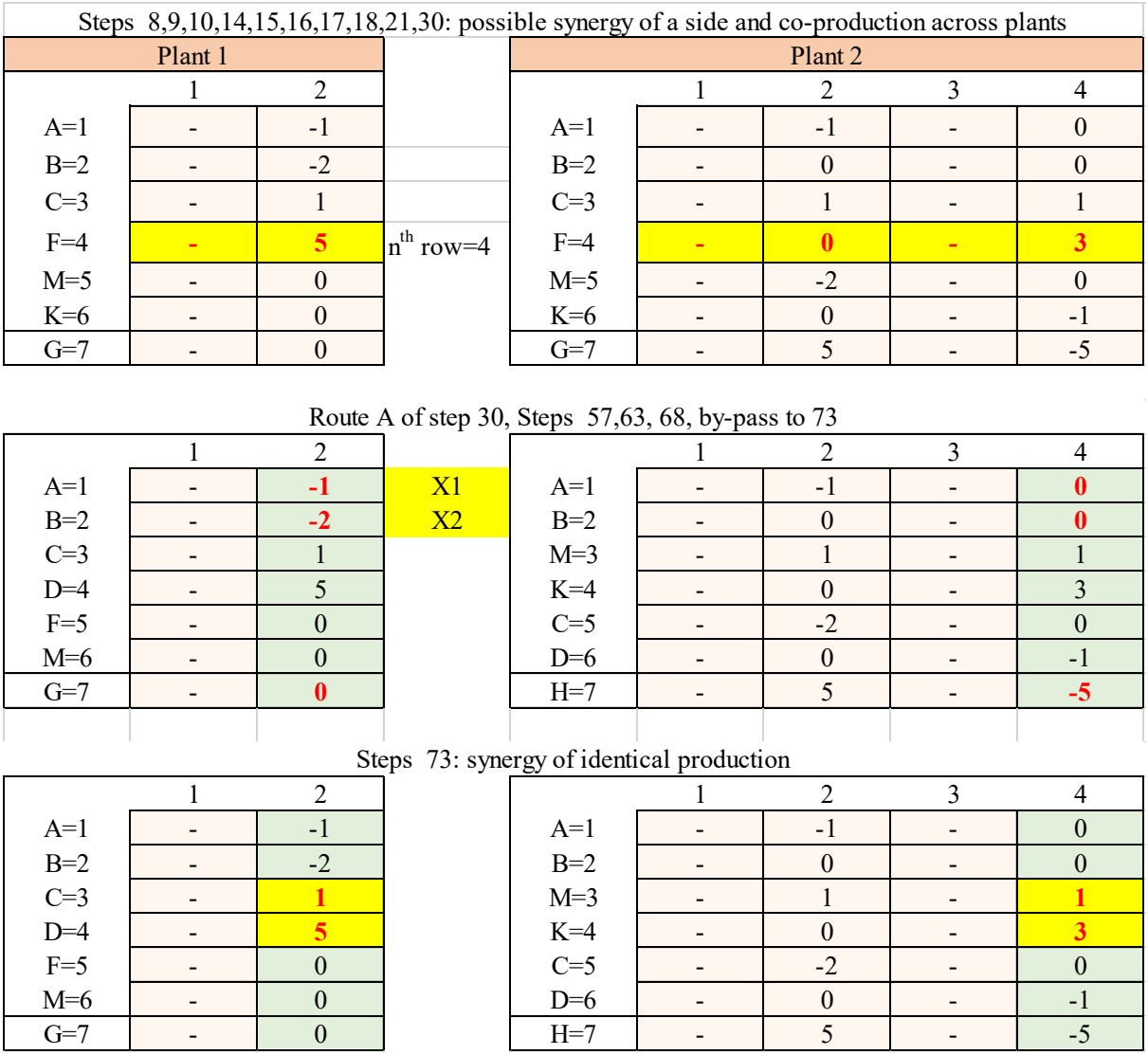
	1	2	
A=1	-	-1	
B=2	-	-2	
C=3	-	1	
D=4	-	5	Y1
F=5	-	0	
M=6	-	0	
G=7	-	0	Y2

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

Figure III-22: Encoded Matrix and illustration towards synergy identification of Hypothetical Example 6, part 2

Solution part 3:

Reference Figure III-23. In the third round, the fourth row is detected to contain similar specie, namely, component F. A t step 30, it detects common elements one being side production one plant while being a co-product in the other, while the latter is given among set of option outputs. Then it suggests to further check over the identical production via route A. This is because this option is valid as long as there is at least one case valid. The later steps yield a synergy of identical production, following same terminologies followed earlier.



Plant 1	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
F=4	-	5
M=5	-	0
K=6	-	0
G=7	-	0

Plant 2	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
C=3	-	1	-	1
F=4	-	0	-	3
M=5	-	-2	-	0
K=6	-	0	-	-1
G=7	-	5	-	-5

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

	1	2
A=1	-	-1
B=2	-	-2
C=3	-	1
D=4	-	5
F=5	-	0
M=6	-	0
G=7	-	0

	1	2	3	4
A=1	-	-1	-	0
B=2	-	0	-	0
M=3	-	1	-	1
K=4	-	0	-	3
C=5	-	-2	-	0
D=6	-	0	-	-1
H=7	-	5	-	-5

Figure III-23: Encoded Matrix and illustration towards synergy identification of Hypothetical Example 6, part 3

III.4.3.5 Summary

In this section. The implementation of the systematic approach with respect to the reactor systems is conducted. The basic approach while considering the reactors is that this algorithm flowchart along with

its instructions, actions, input, output etc., do not interfere with the content of the reactor but rather deals with a given reactor as a chemical specie generator. The approach is designed to result in multiple of possible synergetic opportunities such as partially/totally common reactor operations, opposite reactor operation, etc. of which each of them can be used by the design engineer as a new factor that influences the decision making during the design activity. Later, the developed approach is illustrated by a hypothetical example. In brief, this section shows the contribution of this research towards structurally integrate reactors across process boundaries.

III.5 CONCLUSION

This section provides a comprehensive overview about the steps, reasoning theory, and principles used to properly approach the problem of the current research systematically. This goal is achieved by identifying the parameters available within the systems of interests that are multiple plants. These parameters are classified into sets and subsets. Later, these sets are gathered by representing them into matrix form of which every plant participates in the system is represented by a two-dimensional matrix, making up a system of three-dimensional matrix for set of plants representation, Later, the outputs of the systems are identified and defined. These outputs are simply the opportunities of synergy that may be used to properly approach structural integrated design. It is made clear that these opportunities represent factor that influence the design problem and do not provide design recommendations. Later, more specific input is specified to the systems. This input contains numerical representation of the flow of chemical species in a given system. Thus, by this stage, the actual chemical process flow diagram is encoded in a fully defined numerical form. This numerical encoded system is used as the input to the algorithm flowchart. The algorithm flowchart is simply the sequential execution of steps that transform the given input into the desired output. In this work, an algorithm flowchart is designed for each of the separation (distillation systems) and reactor systems. These systems are illustrated and explained with hypothetical example. In brief, this section represents the comprehensive picture about the steps, implementation, and development of the systematic approach towards structural integration across traditional chemical process boundaries.

CHAPTER IV

ILLUSTRATIVE EXAMPLE PART I: STAND-ALONE PLANTS DESIGN PHASE

IV.1 INTRODUCTION

The basic intention behind conducting a case study is to provide a technical evidence to applicability of the developed approach and to verify the validity of the concept. Furthermore, the case study serves as an illustrative example of the use of the algorithms. Because the application of the algorithm requires knowledge about the process flowsheet and the components flow within its streams, plant design traditional phases are followed. Hereby, plant design starts with process description, representation of the process by block diagram and then by process flow diagram, and then operating conditions are obtained for plant simulation that is followed by heat integration, and lastly closes with plant economic evaluation. The following sections provide the details of plant design phases for the two selected plants.

IV.2 SELECTION OF PARTICIPATING PLANTS

Despite the advantage of the developed algorithm flowcharts of allowing the user a trial and error route for plant selection, design engineer experience plays an important role in the initial selection of the processes. Nevertheless, considering the synergy types that are available by the developed approach may further help in plants selection.

For the purpose of this work, the basic selection took into consideration the patented technologies by commercial corporations. This practice assures the validity of the selected technologies in the industrial scale. Two technologies were selected of were seemed to have synergy

IV.3 STAND-ALONE PLANTS: PROCESS FLOWSHEET REPRESENTATION

IV.3.1 Plant I (Acetic Acid Production by Methanol Carbonylation)

IV.3.1.1 History

Acetic Acid is traditionally produced by oxidation of Butanol and light hydrocarbons. Another route of Acetic Acid production is the oxidation of acetaldehyde. BASF Corporation Carbonylation of Methanol to acetic acid. The old technology disclosed in this patent suffers the high pressure. Advancement to this technology has been considered and disclosed in number of patented technologies with milder conditions. These technologies suffer from the excess amount of water that require further drying columns. One technology that used finite amount of water for acetic acid production is disclosed by Simon D. Aubigne, Jeremy B. Cooper, Bruce L. Williams, Derrick J. Watson. (1994) under title of Process for the production of acetic acid in US Patent No. 5,416,237, referenced [20], using a single distillation zone. This process is selected for implementation.

IV.3.1.2 Process Description and block diagram

- Acetic Acid is produced by Carbonylation of Methanol (Reacting CO with MeOH)
- The catalyst Solvent Composition and reaction conditions favors high conversion of Methanol to Acetic Acid ~ 99%
- Acetic Acid Produce is separated by a flash separator from the solvent
- Purification of Acetic Acid product is accomplished by a single distillation column from water and solvent leftovers.

The process can be described in block diagram format as shown in Figure IV-1.

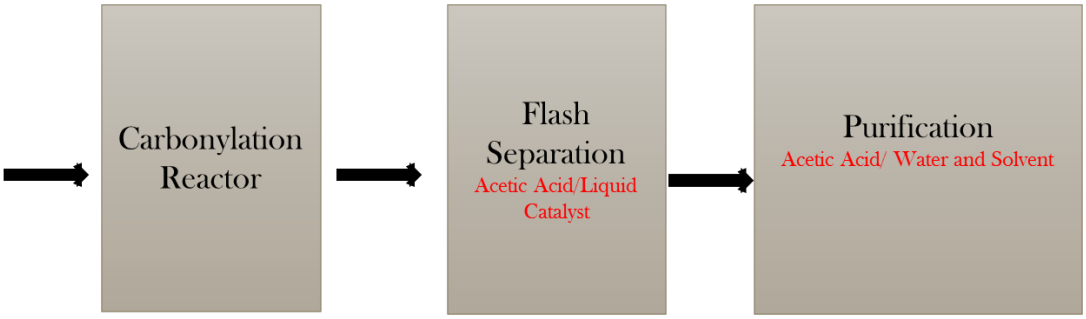


Figure IV-1: Process Block Diagram of Acetic Acid Plant

IV.3.1.3 Process Flow Diagram

The process block diagram is represented with intermediate equipment with more detailed unit operation arrangements by the process flow diagram. The process flow diagram of Acetic Acid plant is shown in Figure IV-2.

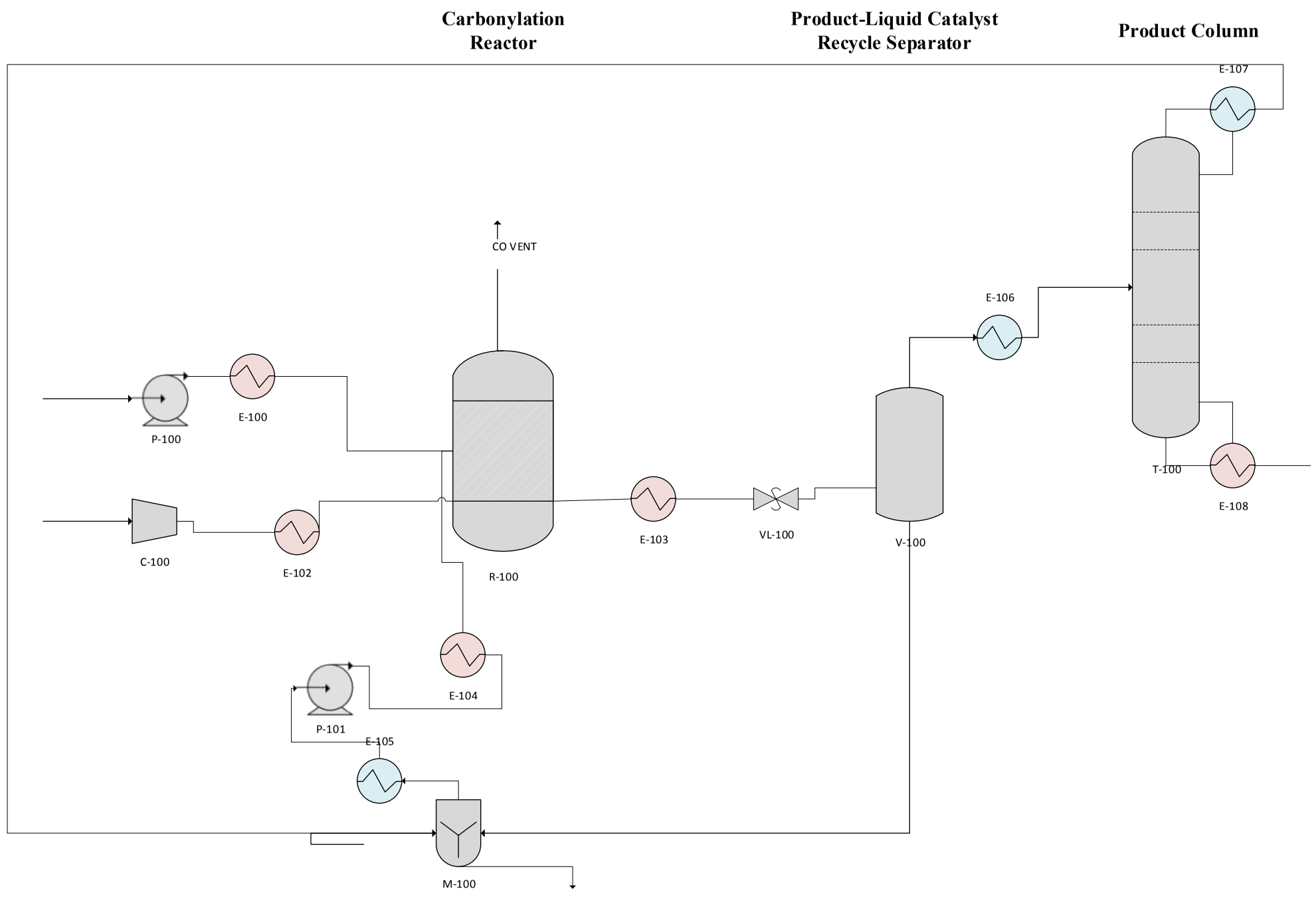


Figure IV-2: Process Flow Diagram of Acetic Acid Plant

Plant II (Ethanol Production from Methyl Acetate)

IV.3.1.4 Brief History

This process is developed by Kummar, R., Taglieber, V., and Schneider, H (1982) for the production of Ethanol from intermediate Methyl Acetate. [21] The technology for ethanol production that is developed by Shuff, A., Torrence, G., Hokkanen, B., Pan, T., Scates, M., and Shaver, r. (2014) [22] is used in this work. It holds the US Patent No. 8,729,318 B1. This technology has main three sections and it is believed to have higher selectivity on the yield of Ethanol than the traditional methods.

IV.3.1.5 Process Description and Block Diagram

- Methyl Acetate and Acetic Acid are produced by Carbonylation of Methanol (CO reacting with MeOH)
- The reaction conditions, solvent composition, and catalyst favor production f Methyl Acetate, conversion ~ 69% of MeOAc, while ~19 AcOH (as simulated and calculate din this work)
- In a flash separator, products are separated from solvent
- Purification of MeOAc and AcOH is accomplished by a single distillation column
- Bottom AcOH stream (with water) are sent to Esterification section to further produce MeOAc
- Esterification unit required addition of Methanol
- Esterified product is combined with the overhead MeOAc stream from initial purification and sent to MeI recovery unit

- Produced free MeI, MeOAc stream is sent to Hydrogenolysis unit
- In Hydrogenolysis unit, Hydrogen is added
- Reaction effluent (hydrogen and Ethanol, Methanol) are separated to recycle Hydrogen, and send MeOH and EtOH to purification unit
- Product column is used to separate EtOH and MeOH

The process block diagram is shown in Figure IV-3, showing the major blocks/sections in the plant

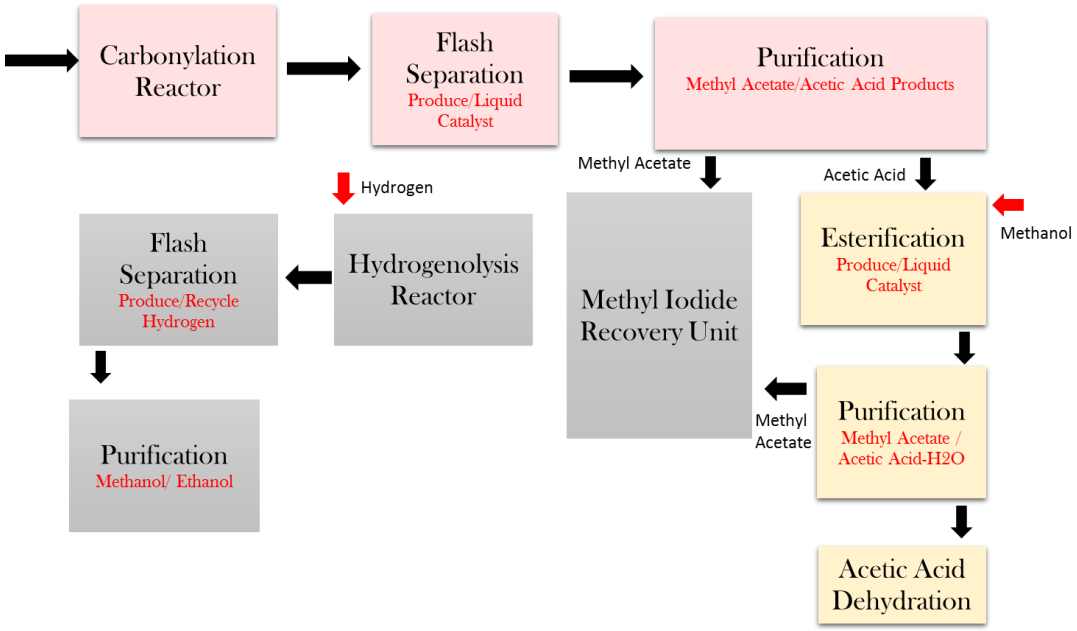


Figure IV-3: Process Block Diagram of Ethanol Plant

IV.3.1.6 Process Flow Diagram

The process block diagram can be represented with detailed flowsheet of equipment and intermediate process conditioners in the process flow diagram. The process flow diagram of Ethanol Plant that is considered in this work is shown in Figure IV-4.

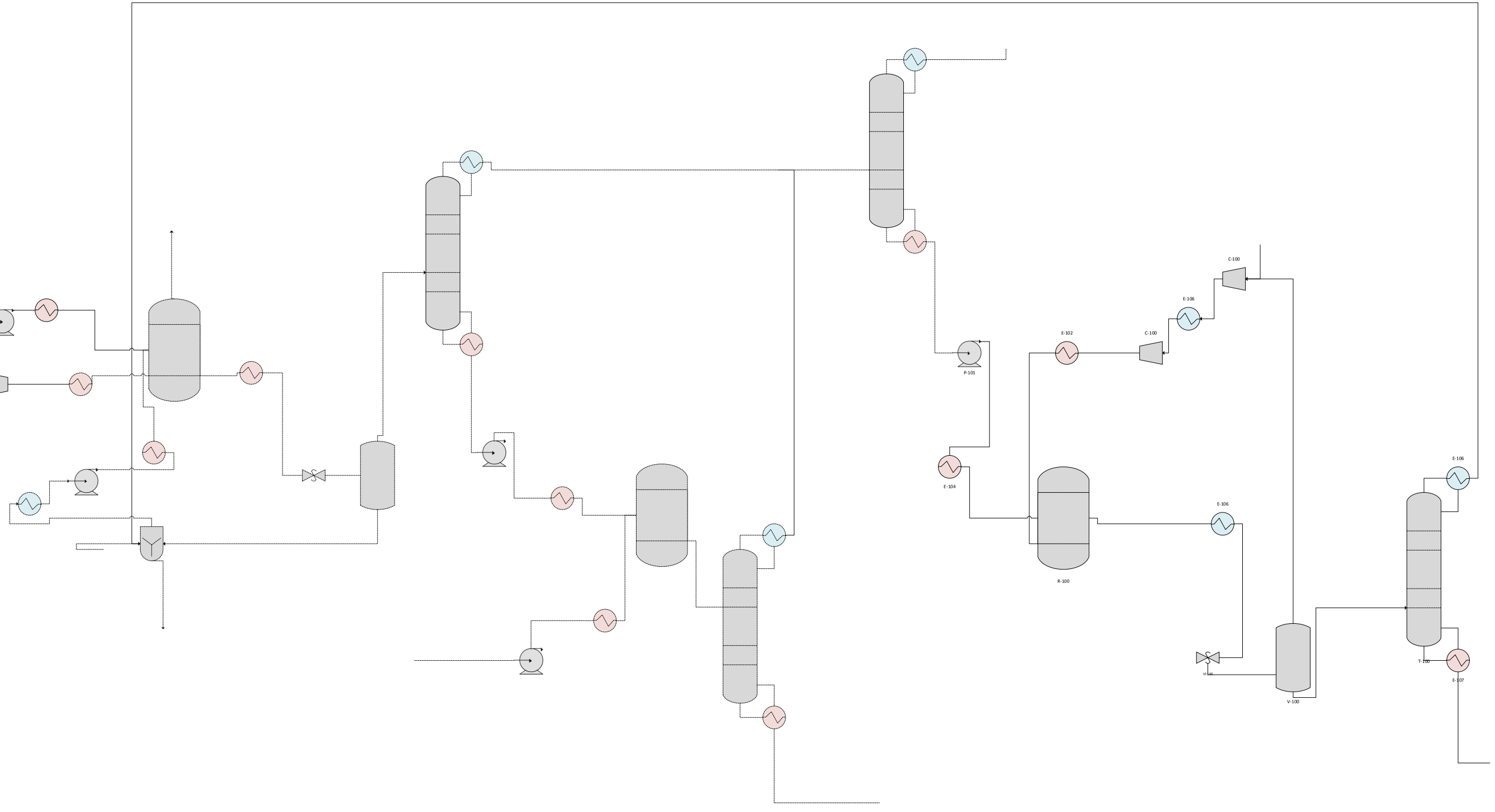


Figure IV-4: Process Flow diagram of Ethanol Plant

IV.4 STAND-ALONE PLANTS: PROCESS SIMULATION

IV.4.1 General Introduction

Chemical process simulation is the act of modeling the process computationally. In the field of chemical process engineering, simulation has undeniable benefits. One benefit is that it provides the design engineer with an experimental environment to develop the process and/or enhance its performance. This benefit is vital since the ultimate objective of a developed technology is to be implemented in an industrial scale which makes the experimentation approach via the iterative actual implementation not a feasible option. Also, this is counted as a benefit over the pilot scale since the scaling up factor is essential to account for many design aspects, for example but not limited to, the number of equipment to handed the capacity in proper intervals and sequence, size of equipment, streams splits, equipment design to handle not only the operation type but also the operation capacity, etc. Equally important, the scale-up factor plays an essential aspect in the act of process economic evaluation as it provides the design engineer with excellent insights and maybe accurate about profitability analysis via accounting for the capital and operating cost as major elements in economic evaluation.

Process simulation achieves the previously states benefits and more since it represents a mathematical model which provide numerical output that is necessary account for process flows, compositions, sizes, costs, etc. The mathematical model that runs the simulated flowsheet and counts its numerical values are known as the Thermodynamic Models.

IV.4.2 Simulation Software Selection

Chemical process simulation software can be classified into two main categories that are SteadyState based, and Steady state and dynamic based. The later type, dynamic based software, in addition to steady state, account for process control. For process flowsheet development, a

steady state model serves the purpose. Aspen Plus™ is used as the simulation software to conduct all cases study parameters in this work. Additional to this, Aspen Energy Analyzer is used to conduct the heat integration of the simulated plants, specifically, for the generation of heat exchanger network.

IV.4.3 Activity Coefficient Models and Equation of States

In this research, Carbonylation sections of both standalone plants as well as Esterification section in Ethanol plant are conducted under the calculations of NRTL Activity coefficient model to account for the polarity with the existing strongly non-ideal mixture. HOC equation of state is selected to account for the non-ideality of the vapor phase. As for Hydrogenolysis section of Ethanol plant, SR-POLAR equation of state is used to account for high pressures and temperatures. The later uses Wilson activity coefficient model to calculate the liquid phase and UNIFAC or HOC for the vapor phase according to Aspen Plus ™ v.8.1. Same application is taken into consideration for the structurally integrated plant.

IV.4.4 Assumptions and Considerations for Simulation

IV.4.4.1 Introduction

The overwhelming approach that is taken into consideration while conducting the case study is consistency. Consistency is an essential factor for cases of where comparison between different elements is required. In the context of process simulation, consistency can be appreciated as providing the same level of accuracy, degrees of freedom, implementation approach and method etc. This is essential in order to assure that the overall comparisons are valid. In order to achieve the global goal of consistency, every unit operation type had number of assumptions and considerations that are applied to all conducted cases in this study.

IV.4.4.2 Reactors and Reactions

The simulation of reactors suffers number of limitations. In nature, reactions take place whenever the conditions for their accordance present. However, RStoich Model in Aspen Plus is unable to predict the chemical changes of the present chemical species under specified conditions unless the reaction is specified as it execute what is being specified regardless it is possible in reality or not. For example, if for given conditions, a side reaction takes place in nature, however, Aspen Plus does not account for it if it is not specified. Thus, careful attention is considered when making execution assumptions in the reactor units. In addition, the catalyst composition and type that influence the reaction (s) conversion and selectivity if applicable, cannot be specified, rather, the conversion and selectivity direct input are used to mimic the catalyst performance. Finally, the reaction system whether it is parallel, series, or both (i.e. complex reactions) are not easily manipulated by the use of Aspen plus, may require advanced details about the kinetics such as the rate of reactions, order, mechanisms etc. As a general background, the term chemical reaction refers to the change in chemical and subsequently physical properties when a reactant is being converted into a product with a change in chemical bonds. The factors that determine the conditions for a chemical reaction to occur are significantly a lot. In chemical engineering, reactions are classified into two main categories, kinetics and thermodynamics. In principle, chemical reactions are either thermodynamically controlled or kinetically controlled. To know to what extent products are at given conditions may represent the aim of conducting equilibrium analysis. [17] On the other hand, answering the question of how fast the reaction proceeds is the field of reaction kinetics. [17]. Each of these fields, determine factors to identify the nature of chemical changes for chemical species. What may make the situation even more critical is the lack of information in the simulated technology references. This is simply because the overwhelming

objective of these references is to present the novel technology which referred to other references in the details 70 of kinetics sometimes. Thus, degrees of freedom should be evaluated to assure that the system that is to be applied is solvable. Because of the preceding arguments, careful application of reaction conditions in simulation is considered. The decisions/assumptions that are made while simulating reactors in this work can be summarized by the flowchart shown in Figure IV-5 which takes into account the available information of the simulated technology**. Otherwise, if operating conditions ranges are available, an assumption of using data within the ranges maybe made.** Generating this flowchart is essential in this study for number of reasons: 1) following this chart assures that all conducted examples are executed on same basis and reasoning, 2) It resolves the problem of repetition in the sequential instructions for different cases that end up with same assumption, and hence enhance simplicity, 3) it illustrates the arguments in an easy-to follow way, and can be easily be considered to evaluate the significance of the taken assumptions for later steps evaluations of this work, i.e. economic evaluation.

In the use of this flowchart, some definitions are made clear for the presented instructions as follows:

b. Color code blue refers to the need of using a reference that is other than the original reference. In this context, an original reference is defined as the reference of the simulated/applied technology. Despite that it is most preferably to use all information from the original source, in case of lack of information, other reliable references may be used. In this context, the adjective *reliable* refers to a reference that satisfies ALL following conditions:
    i. The temperature value(s) of the used reference flows in the same range as the original reference

ii. The pressure value (s) of the used reference flows within the range mentioned in the original reference

iii. If catalyst present, evaluation of the used catalyst active phase, promotors, and carrier should be done. Differences in compositions and/or type of any can be ignored only if it is evident that these differences do not have an adverse effect on the reaction performance (conversion, selectivity, etc.).

iv. The component of the solvent, if applicable, should be the same, and if any differences present, it can be used only if it is evident that this difference does not have an adverse effect on the reaction performance (conversion, selectivity, etc.).

v. As general limiting role for conditions iv and iii, if catalyst AND solvent present in the technology of original reference, catalyst AND Solvent should present in the used reference.

c. Color code orange refers to the need of stating assumptions that may be obtained/concluded from other reliable references as defined in the preceding section or may be obtained from conclusions/calculations made out of leading information that act as implicit source of the information of interest within the original reference. As a special case, the assumption of dropping a side reaction should be carefully made, considering the following:

i. It can be totally ignored if the original reference as defined in the preceding section allows to drop it or had dropped it in any embodiment of the study including illustrative examples.

ii. If point I is not applicable, the

iii. reaction can be dropped under a condition that it should be revisited when structural integrated approach is applied.

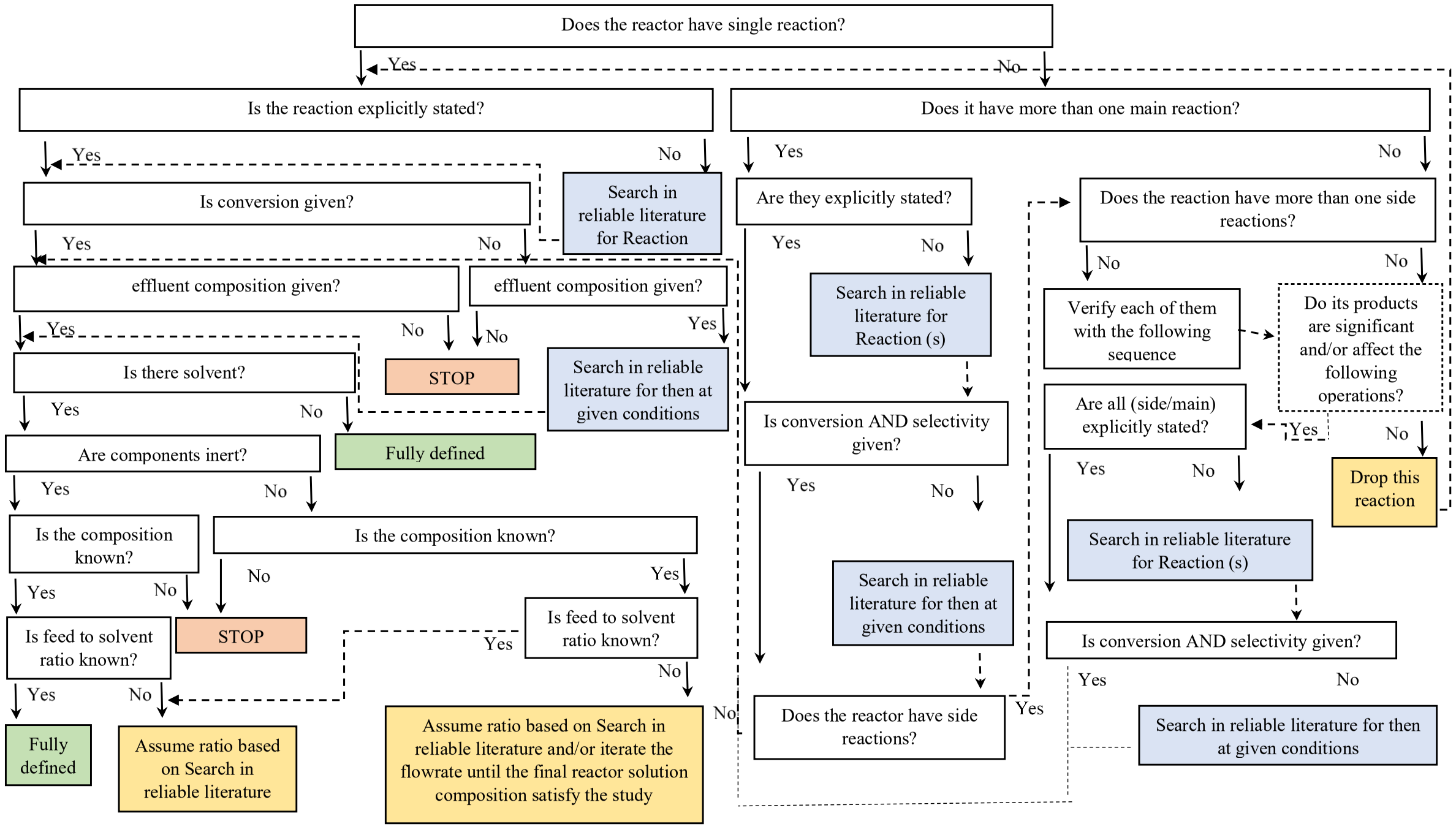


Figure IV-5: Flowchart of Reactor Simulation Guide designed for the purpose of this work

IV.4.4.3 Distillation Columns

DSTWU Model that is known as short-cut method, employing Fenske-Underwood-Gilliland method to calculate the minimum reflux ratio and number of stages is used provide an initial guess for the operating conditions. Slight further modification on operating conditions by are applied if DSTWU obtained parameters do not converge in RadFrac rigorous model

In case of Azeotropic separation, trial and error approach is used until separation is performed because DSTWU does not solve for Azeotropic mixtures. Also, Azeotrope type maybe selected in some cases.

IV.4.4.4 Flash Separators (Equilibrium Separation)

- In presence of gases, cooling is given priority prior to the flash separator.
- For liquid separations, manipulation of temperature and pressure are performed by trial and error/sensitivity analysis until desired product is separated

These conditions hold unless otherwise particular specifications are given by the technology that is simulated.

IV.4.4.5 Heating and Cooling

- Pressure drop is specified following heuristics. Heuristic rules followed as per to [9]
- Segmentation (number of heat exchangers in series) is not considered in the basic implementation of the flowsheet in order to minimize constraints for the heat integration step of which segmentation would take place, favoring heat integration options.

IV.4.4.6 Compressors

- Segmentation of compressors is followed according to heuristics based on pressure ratio
- Intercoolers temperature and pressure drop is defined following heuristics

IV.4.4.7 Feed conditions

To fully define a stream, information about temperature, pressure, composition, and flow rate are needed. The raw materials used to feed the processes are supplied at given conditions as per to the transportation system. Although the phase (vapor/liquid/solid etc.) of a given chemical or mixture of chemical varies with the conditions (pressure, temperature, etc.), hereinafter, chemicals that present as liquid at ambient conditions are referred to as liquids while the ones that present as gases at ambient conditions are referred to as gases. Specifying the feed temperature and pressure should be done carefully since, especially for gases, affect the utility cost and capital cost required to bring the material conditions to the process conditions. In default, liquids are stored in storage tanks at ambient conditions, specifically 298 K and 1 atm for temperature and pressure respectively. Hydrogen enters as a feedstock at 15 bar with 323 K while CO at 298 K at 10 bar, taking into account molecular size. It shall be understood that these are assumptions/approximations that is made by the author if this work.

IV.4.5 Simulation of the Plants

IV.4.5.1 Plant I (Acetic Acid production by Methanol Carbonylation)

The simulation of the process is divided into sections of where each section may include several simulation procedures and assumptions. For plant I, namely the process of AcOH via MeOH Carbonylation as illustrated by [20], is divided into sections. Referring to the PFD as shown earlier in this work, the first section is the Carbonylation reactor, consisting of feed Mixer, reactor, flasher/phase equilibria separator (with intermediate pressure changer and heat exchanger) and solvent recycle. Also, the separated unreacted gas/methanol recycle that appears in this section is added at the last stage of the simulation. The second section is the purification and recycle section. In this section the crude AcOH as being purified to AcOH product and overhead recycle stream back to the reactor.

Section I: Reactor

According to the flowchart in Figure 8.5, first step is conducted to sort out the involved reactions in a given reactor. Production of acetic acid by the Carbonylation of methanol can be represented in the following reaction

$$CH_3OH + CO \rightarrow CH_3COOH$$

This reaction is not stated explicitly in the used reference. Knowing that the Carbonylation of methanol may undergo other reactions, a review on disclosed information in [20] is done to assure whether side reactions occur under their used catalyst and applied conditions. The first side reaction that is detected is the water gas shift reaction (WGSR). The presence of hydrogen may be a result from WGSR or as part of the feed with a restriction to partial pressure of 150 psi. [20] The second one, although not explicitly stated in the used technology that is related to the production of propionic acid by-product. A concentration specification of less than 500 ppm in the acetic

product stream is specified by [20]. Thus, a literature search is conducted to figure out information its production of propionic acid in the context of Carbonylation conditions.

1. Water Gas Shift Reaction

   In principle, WGS reaction is a reversible reaction as shown below. “The reaction is equilibrium limited, and the equilibrium constant varies with temperature”. [23] Although the conversion of this reaction is not explicitly stated, one information mentioned helps to figure out a limit for the conversion. “Hydrogen present in the reactor as a result of the water gas shift reaction and optionally as part of the gas feed is preferably maintained at a partial pressure of at least 2 psi, preferably up to a maximum partial pressure of about 150 psi” [20], p.3. Thus, the conversion of the reaction should be adjusted not to exceed this limit of Hydrogen Partial pressure. However, due to lack of information relate to material balance section, this reaction is omitted.

$$CO + H_2O \leftrightarrow H_2 + CO_2$$

2. Propionic acid by-product, EtOH Carbonylation

   In the process, MeOH feed impurity of EtOH, the reaction of EtOH with CO, producing propionic acid as main liquid. [24] By checking back the flowchart of reactor simulation, the conversion need to be found. Since it is not mentioned in [20], one approach was followed. The final concentration pf Propionic acid is mentioned, being constrained with a minimum level of MeOAc liquid reaction composition. Thus, one approach is to adjust the impurity of EtOH in the feed was exceed side-production of Propionic Acid limit. However, this approach assumes full conversion of EtOH. This assumption is made since no EtOH present in the reactor effluent according to [20] of interest, and hence, and EtOH

essentially present as Propionic Acid. Due to these arguments, the side reaction of propionic acid is omitted din order to avoid wrong execution of the reactions chemistry. Also, this assumption is considered to be acceptable since this technology claims that it produces low concentrations of this impurity with no need to additional purification units. Hence, by following the guide developed and shown in Figure 8.5, this reaction can be omitted.

Other side reactions found in the literature are as follows.

For practicality of the conducted study, as a product of AcOH traditionally suffers the production of dimethyl ether and methyl acetate lowering AcOH yield, a search for other references in the literature is conducted. According to [25] the following side reactions b and c are combined with the main reaction a.

$$CH_3OH + CO \rightarrow CH_3COOH\ (a)$$

$$CH_3COOH + CH_3OH \rightarrow CH_3COOCH_3 + H_2O\ (b)$$

$$2CH_3OH + CO \leftrightarrow CH_3OCH_3 + H_2O\ (c)$$

Now, according to the flowchart, the reference of these reactions need to be verified in terms of the applicability to the original reference [20]. Following the four main rules listed earlier for the use of references in the context of reactions, the following check is made:

According to [25] (supporting reference), the following conditions are satisfied, approving the use of it for the original patent as a reliable supporting reference:

1. The process is the same, that is titled process for the production of Acetic Acid from Methanol and Carbon monoxide using supported Rhodium catalyst
2. Temperature range, is 140 C to 250 C.

3. Pressure range, ≅ 15 to 60 bar
4. Catalyst: Rhodium is the active phase and Methyl Iodide is used as a promoter
5. Solvent restrictions of water content, 0.5 – 10 wt%. For the solvent, the extent composition is used in a closed extent of similarity between the two studies since the supporting reference presents varies example of which a close one is picked for the use of information.

Thus, two side reactions can be added that are b and c for the side reaction of MeOAc and DME respectively. Hereby, flowchart for reactor simulation moves to the question about conversion and selectivity. Since conversion nor selectivity's in [20], up to the review of the author of this work, are explicitly stated, it should be figured out either by a leading information within the work or by reach in a reliable literature as defined earlier. Fortunately, an information about the conversion could be obtained. In example 1 of [20], the feed mass flow and AcOH product flow is provided in pilot scale. However, due to the absence of the previously stated side products in this example of the referenced patent,[20], these side reactions are omitted.

The following points summarize the steps/decision and assumptions taken to achieve the needed conversion values and the overall mass balance. A comprehensive mass balance tables at the pilot scale and the industrial scale are available in the Appendix B.

Needed Information:

1. Overall conversion of MeOH to Acetic Acid

2. Solvent to Methanol feed ratio

This information may be subjected to the flowchart of Figure 8.5 to obtain the following:

1) Reactor effluent composition, named, reaction solution in [20], is given.
2) The feed to distillation column in volumetric flowrate is given
3) The bottom product of Acetic Acid of distillation column is given in mass flowrate
4) the feed of CO and MeOH are given in mass flowrates.

First assumption: Conversion of MeOH to AcOH is 100% since no MeOH is reported in the effluent by the original reference [20], this assumption is considered. More precise understanding of this can be provided by following the whole set of assumptions presented here.

Second Assumption: Conversion is calculated based on the feed of Methanol versus product of AcOH given. Because the product of AcOH value is taken from the value of AcOH removed from the bottom of Distillation column in the later steps of the process, two cases are valid to validate this assumption. Case 1: if AcOH recovered from distillation has quantities of AcOH of te solvent, the calculated conversion will be overestimated, while Case2: if the AcOH recovered from distillation is a result of loss in quantities due to the separation, the calculated conversion is underestimated. In both cases, it is not expected that these deviations are dramatically to affect the process performance assuming recovery up to a very good extent of AcOH.

Third assumption: The composition given in [20] of reaction solution is illustrated in Appendix B under title of reaction solution composition. Modifications is made to account for the catalyst stabilizer (slat used) in the salt compound rather than ions. Thus, Lithium and Iodide are added to give Lithium Iodide salt overall composition. It is worth mentioning that "0.55 wt % lithium (present at least in part as iodide salt) and 11.6 wt % iodide " [20] p. 9. The entire composition is normalized.

Fourth assumption: The conversion of Hydrogen Iodide that present in the distillation zone to Methyl Iodide by addition on Methanol is omitted. Description about this is available in [20] while addressing hydrogen iodide presence in the feed and its buildup drawback, it mentions information to convert the hydrogen iodide to methyl iodide This assumption is expected to adversely affect the economics of the process since it does not require extra operating units + feed of raw material Methanol is little relative to the former feed.

Fifth assumption: the mass flowrate of Methanol given in the feed is noted in a footprint comment at the composition table as including methanol feed to distillation. According to assumption 2, this conversion is omitted and hence the amount included for Methanol in the feed is omitted.

Sixth assumption: following assumption 3, the amount of Methanol feed to distillation is given in Table 2 in [20] as 55 g/h. Thus The feed to the reactor results in 1.26 kg/h - 55/1000 kg/h = 1.205 kg/h methanol feed to Carbonylation reactor. However, if this is the right understanding of the original reference, this Methanol feed, 1.205 kg/hr to result in 2.33 kg/h AcOH results in a conversion that is higher than 100%. This may be acceptable only in case AcOH in the solvent is being removed with the product, increasing the production. Thus, feed of Methanol is taken to be the entire amount mentioned in table 1 of [20].

Seventh assumption: Feed to solvent ratio is basically taken as initial guess to be 1 to 2.9 mass ratio. This initial guess is made from the Carbonylation reactor of Ethanol plant of this study. It is true that the compositions of two solvents are different (which makes them different targets processes) but an initial guess of a ratio, considering the compositions are known, is considered to be a valid option.

Eighth assumption: Assumption 6 will be validated for a final feed to solvent ratio after separating the AcOh product with the given conditions, the water mass fraction should be less than 8%, assuring the assumption since H2O exist in the solvent and does not participate in the reaction.

A check is made on the simulation data sheet: water mass fraction is around 2% which means that ratio of solvent is valid.

Ninth assumption: CO is assumed to be vented 100% from the top of the reactor since its composition does not present in the reactor solution given in the reference.

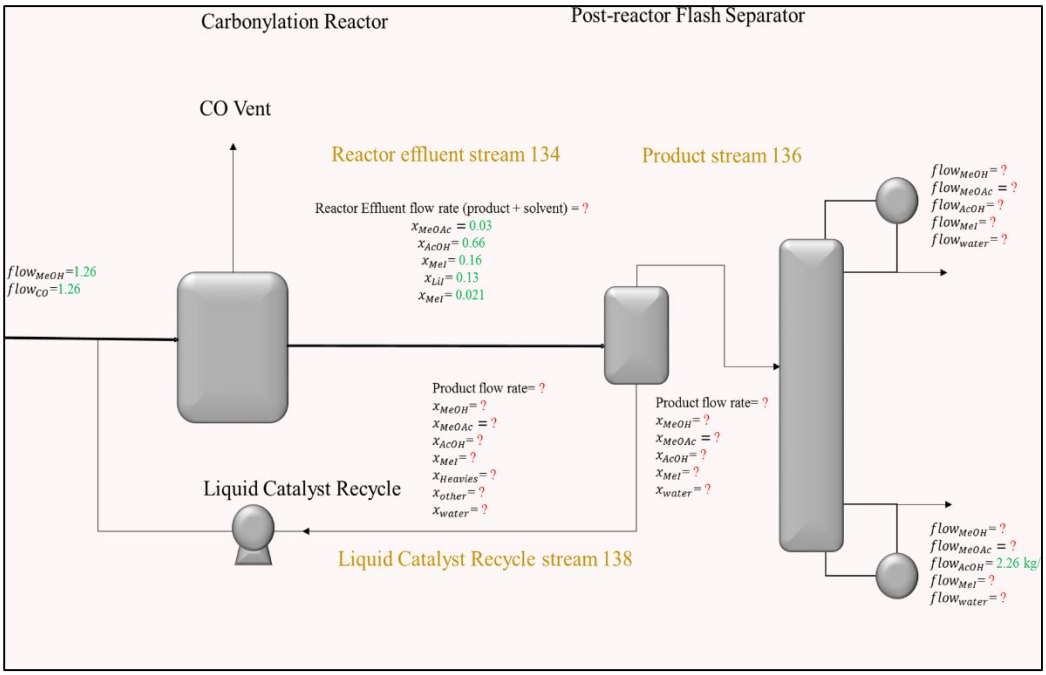


Figure IV-6: Material balance for Carbonylation reactor at Acetic Acid plant

How material balance is conducted? The following steps refer to Figure IV-6 and mass balance table of Carbonylation reaction in the Appendix B.1

1. according to assumptions 4 and 5, Methanol feed is calculated from molecular balance based on AcOH production, and hence it is known

2. CO is already in excess

2. Reaction Solution mass composition is obtained from the table of reaction solution composition, Appendix B, of this sheet, according to assumption No. 2

3. According to assumptions 6 and 7 , feed to solvent mass ratio is 1 to 2.9. Thus, the flowrate of solvent catalyst solution is known (solvent without AcOH produced)

4. According to assumption 8, CO outlet stream is known.

5. Since AcOH produced flowrate is known and Solvent flowrate is known, a balance is conducted considering that: Reactor effluent Acetic Acid Produced + Solvent in the system.

Material balance tables can be found in Appendix B.1. These tables are conducted based in the assumptions and reasoning of this section.

Section II: Purification

The prettification/separation unit of Acetic acid plant followed number of steps for execution. These steps are illustrated in the following points:

1. DSTWU Column model is installed in order to get initial operating conditions of the column. The recovery specifications are as the following:

2. Since the production capacity is calculated in a reverse manner, starting from the recovered AcOH from bottom of distillation, almost full recovery is desired. Thus it is specified as 99.5%, considering that 2 to 3 moles may be lost out of 640 (base case capacity example)

3. Water recovery in the TOP stream should be nearly perfect since in table 3 of [20], water exist in ppm levels in the AcOH stream. i.e. above or equal 99.9%

4. Key components are AcOH and water

5. The top stream is recycled to the solvent

Considerations for the purification column:

1. The vapor product of flasher is condensed before being sent to distillation column since reference [20] mentions that this stream is being condensed.

2. The overhead of distillation column is recycled to reactor as per to the understating of the referenced patent [20]. this recycle saves solvent material. however, in this work, cost does not involve solvents.

By simulating the purification section, the overall flowsheet simulation of Acetic Acid plant is wrapped up. Figure IV-7 shows the simulated flowsheet. Mass balance, operating conditions, and stream data are available in Appendices B, C, and D respectively.

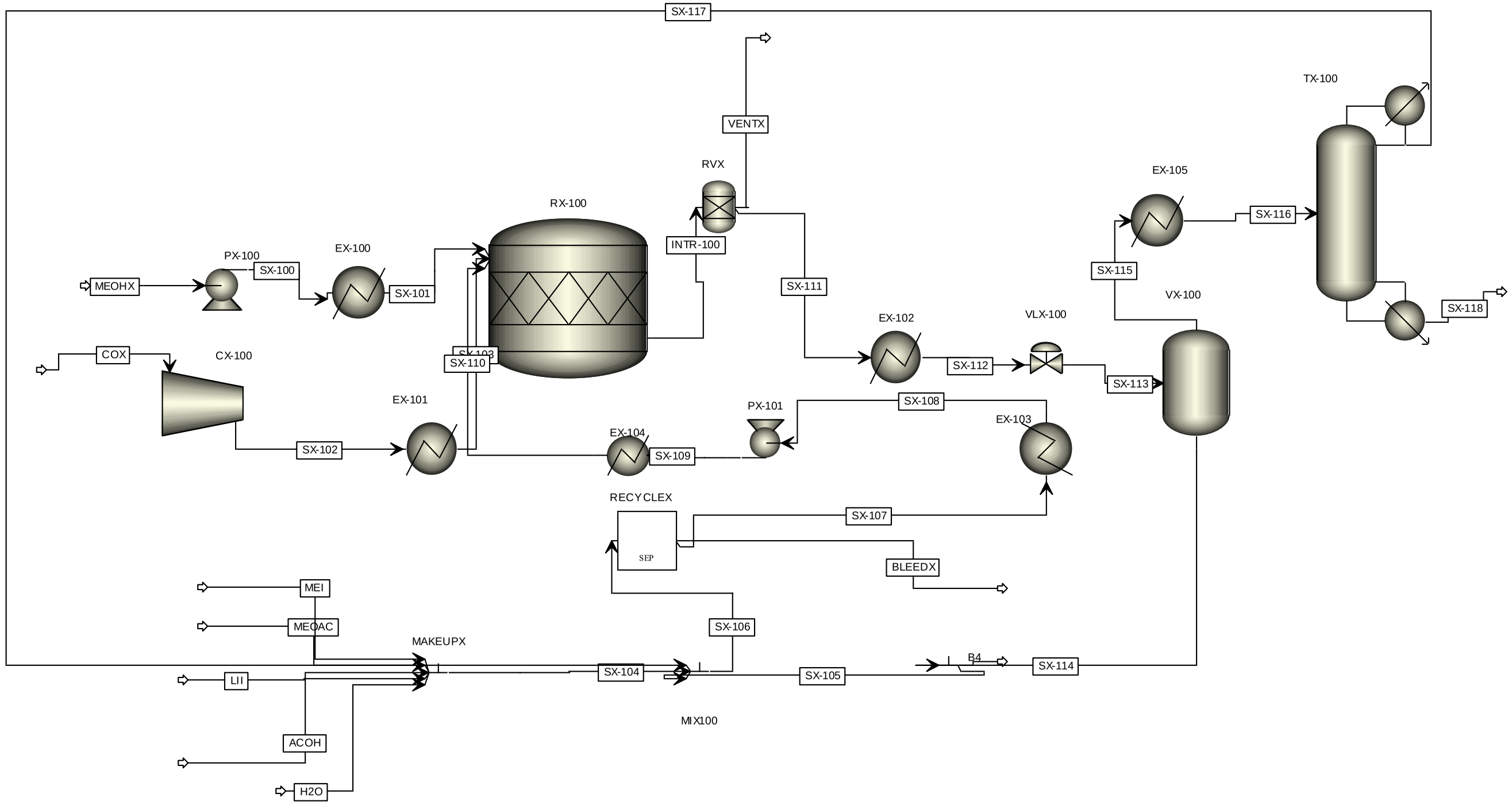


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Figure IV-7: Simulation Environment of Acetic Acid Plant by using Aspen Plus ™

IV.4.5.2 Plant II (Ethanol Production from Methyl Acetate)

Section I: Carbonylation of Methanol

The following points summarize the needed information:

1. Overall conversion of MeOH

2. Selectivity towards both MeOAc and AcOH

Possible solutions

following alternatives are generated accordingly:

1. Use of the available Information by [22]

1.1 Reactor effluent composition (stream 134) and separated product composition (stream 136) as shown in the figure of this sheet

1.2 Deviation from the exact composition should be reasonably justified and other ranges to be used for further decision making

2. Use of supporting reference

By following the set of rules listed in sheet "Set of rules for the use of a reference)

Since this section encloses chemical changes (chemical reactions), a reactor present. Since a reactor present, the developed approach to simulate reactors is followed. First, the reactions involved in the system should be identified. By the reference of the main technology, methyl acetate is formed by Carbonylation of methanol using alkyl halides. A portion of Methanol is related to produce Methyl Acetate by reacting with Acetic Acid solvent. [22] Since these reactions are stated explicitly, they can be obtained as reactions obtained from [26] as follows, describing that based on the used solvent, Methanol and Carbon monoxide react as follows:

$$CH_3OH + CO \rightarrow CH_3COOH \qquad H_2O \text{ Solvent}$$

$$2CH_3OH + CO \rightarrow CH_3COOCH_3 + H_2O \qquad CH_3OH \text{ Solvent}$$

In the simulation these two reactions are considered as the main reactions.

Since esterification is explicitly stated to take place in the Carbonylation reactor as just cited above. It is represented by the following reaction:

$$CH_3OH + CH_3COOH \rightarrow CH_3COOCH_3 + H_2O$$

The reactor specifications of the technology are given by [22] and classified in table below

Table IV-1: reactor range specification by [22]:

Reactor 114 specifications	Conditions/description	Page number
Temperature, C	Preferably 150 – 250 150- 225 150 - 200	9
Pressure, MPa	Preferably 1 - 20 1 - 10 Most preferably 1.5 - 5	9
Catalyst active phase (metal)	Catalyzed, e.g., rhodium-catalyzed	8
Catalyst Promoter	Methyl Iodide	4
Solvent (component/composition)	It is preferred that the solvent includes pure or mixtures of an alcohol feedstock, and/or the desired carboxylic acid and/ or esters of these two compounds. Acetic Acid and Methyl Acetate are preferred solved reaction medium for the Carbonylation reaction of low water content.	9
Conversion/selectivity	No mentioned or at least not explicitly mentioned	-
Other restrictions	Water concentration in the reaction medium up to 14%	9

According to Table above conversion nor selectivity are available or at least not explicitly available for the Carbonylation reactor. Three conversion/selectivity information (for three reactions) correspond to Methanol conversion and it acts as the limiting reactants in all reactions. In order to find out the missing information of conversion and selectivity, number of approaches can be taken. Before stating them, material balances around the system of interest is conducted by the use the available information. Then, extent of reaction system of interest setup is illustrated. After obtaining all possible obtainable material balance values by the original reference, two main

approaches are conducted. The first approach uses stoichiometric relations between reactant and product to find out conversions. The second approach is represented by obtaining the missing information from a supporting/reliable reference as defined earlier in this work. The approach that results in more reasonable values/assumptions is considered for the simulation. These two approaches are reported in detailed in the following two sub-section.

Extent of reaction setup

Before conducting extent of reaction balances, it is essential to check the dependency relations between these reactions (the three reactions identified earlier). This can be done by re-arranging them in a matrix and perform any suitable elimination method, i.e. Gaussian elimination. This attempt is illustrated below:

Thus, the following three reactions should generate five equations since five components are participating in these reactions. They are re-listed here again:

$$CH_3OH + CO \rightarrow CH_3COOH$$

$$2CH_3OH + CO \rightarrow CH_3COOCH_3 + H_2O$$

$$CH_3OH + CH_3COOH \rightarrow CH_3COOCH_3 + H_2O$$

First, the reactions are re-arranged and equated to zero:

$$CH_3OH + CO - CH_3COOH = 0$$

$$2CH_3OH + CO - CH_3COOCH_3 - H_2O = 0$$

$$CH_3OH + CH_3COOH - CH_3COOCH_3 - H_2O = 0$$

$CH3OH$	CO	$CH3COOH$	$CH3COOCH3$	$H2O$
1	1	−1	0	0
2	1	0	−1	−1
1	0	1	−1	−1

By Gaussian elimination, the following matrix is generated, showing the dependency between the third and second reactions:

$CH3OH$	CO	$CH3COOH$	$CH3COOCH3$	$H2O$
1	1	−1	0	0
0	−1	2	−1	−1
0	0	0	0	0

In this case, if one reaction is to be eliminated so that the other two independent reactions fully represent the system and compensate on the elimination of the third reaction, the new generated stoichiometry must be used. However, the new stoichiometry generates different sets of reactant and product for the second reaction. Although the new generated reaction based on the new stoichiometry is molar balanced i.e. components in = components out, yet it cannot be used because it does not represent an actual reaction in the chemical reaction sense. Thus, as an assumption, the overall conversion will be considering two reactions, and the individual reactions conversions (selectivity) is calculated based on the real stoichiometry with just assuming the third reaction does not exist as a solution to this issue. This assumption does not impact the overall conversion; however, it may impact the selectivity. Yet, it is still considered as an assumption. The validity of this assumption is considered to be weak in comparison to the alternative of extracting the data from the original reference [22].

Reverse calculation to figure out the conversions is conducted as the following:

Assumptions:

1. CO Vent is separated in 100%. By an agitator, carbon monoxide of the gas phase is dispersed throughout the reactor.[22] Also, this assumption is made since no explicit CO composition in given in the effluent in the reactor.

2. The components defined under Heavies are appreciated as Lithium Iodide (mimic the catalyst stabilizer, since Rh component cannot be converged in aspen plus.)

3. Product stream is assumed to represent the production of the reactions in 100%

4. The components termed as Others are assumed to be 0, and hence the balance that is 99% is normalized. This assumption is made since if other species exist, no knowledge about them nor their reaction is available.

Procedure to solve the material balance: (Reverse calculation approach)

1. By making a balance around the flash separator, if basis is given to the feed stream to the flasher, namely stream 134, then the flowrates of the two product streams of the flasher, namely, streams 136 and 138 can be calculated by flash calculations restricting the overhead compositions

2. Aspen Plus ™ is used to conduct the flash calculations. Sensitivity analysis is performed by varying pressure and temperature. The following sub-procedure is taken into account while deciding on close available options by sensitivity analysis:

2.1 Temperature and pressure were varied over a range of 1.5 to 15.5 bar and 150 to 240 C respectively. The former is restricted in this range to converge with the Equation of state, while

the latter is restricted by the maximum allowable temperature by the reaction medium, which is assumed to assure the molecular stability of components since it is already specified by the original reference.

2.2 The recycle stream may contain methyl acetate as well as an amount of Acetic Acid may be lost in it. [22]

Accordingly, it is assumed that a greater portion of acetic acid is lost in the solvent, and less of Methyl acetate

When selection upon available options, the set of compositions that have roughly close deviation from the available data by the reference is used. This is to make sure that all components are almost fairly deviating from the original data. For example, if MeI is 2% higher than the original data, then MeOAc and AcOH should be deviating approximately around the 2%. MeOH and Water were sort of under estimated.

3. The selected operating conditions were re-plugged in the software, and the resulted stream is used to complete the material balance in this excel sheet. The resulted data of flash is available in The tables of Appendix B

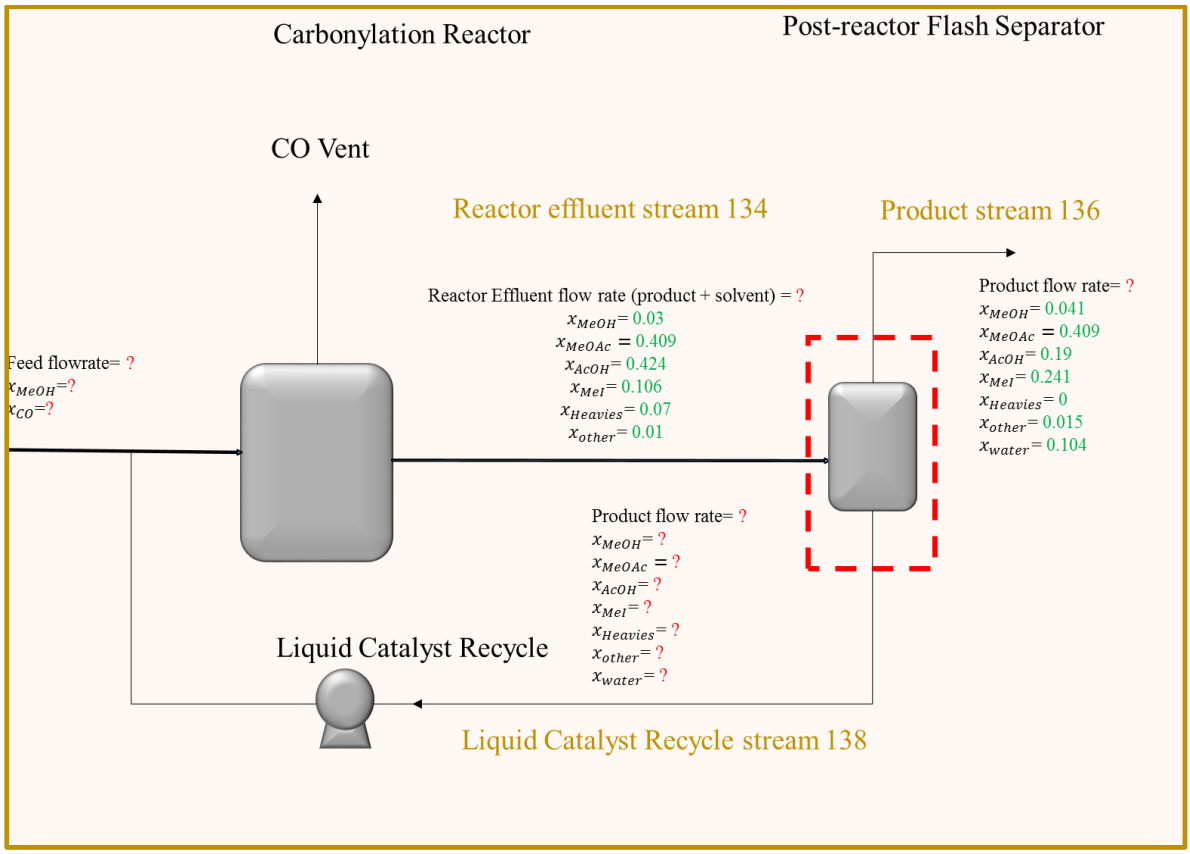

Figure IV-8: Mass balance around the flash separator

Figure IV-.8 above shows the material balance at the Carbonylation reactor section. Also, two pictures are available in Figure IV-9, showing the material balance boundaries around the flash separator.

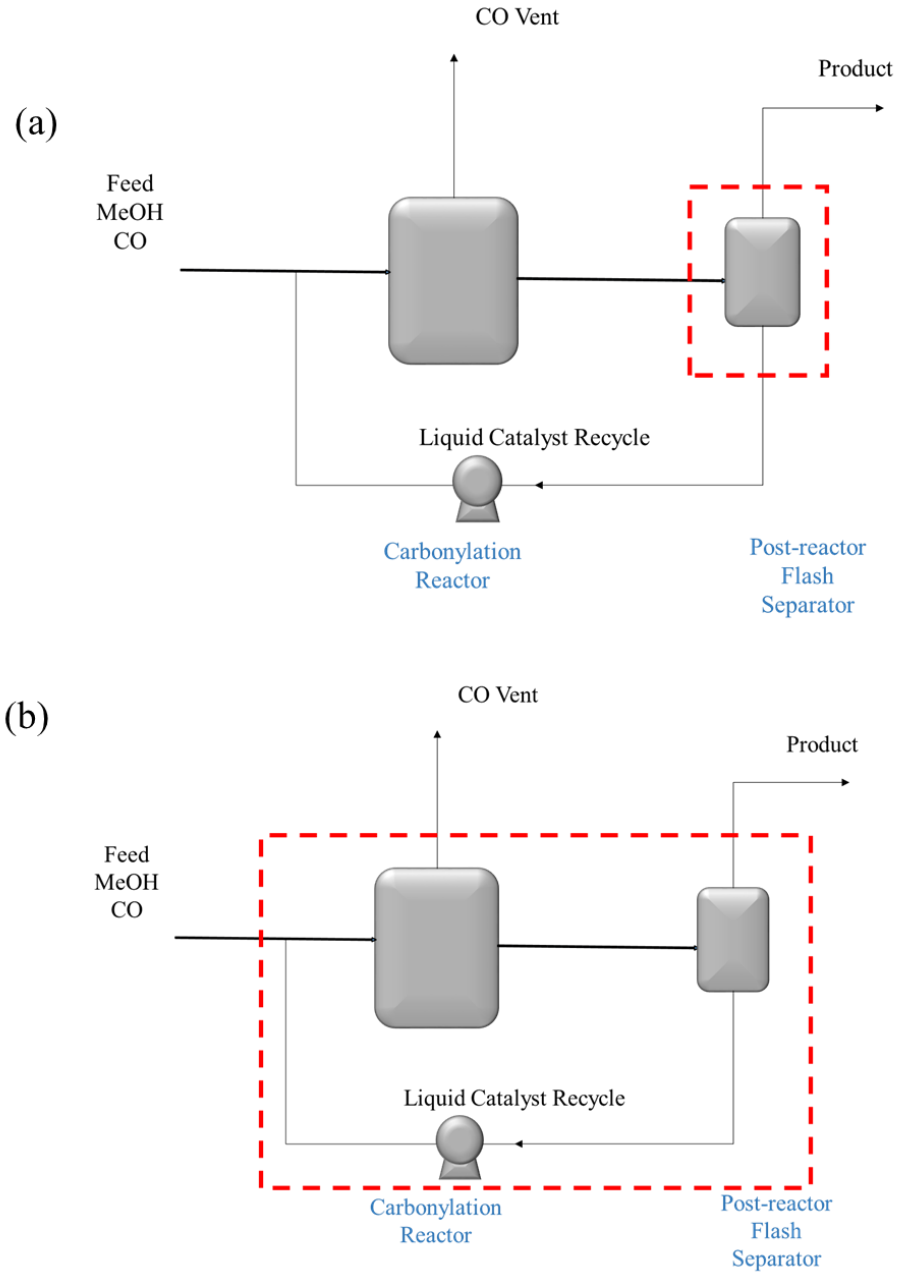

Figure IV-9: Material Balance boundaries visualization around the flash separator and Carbonylation reactor at Ethanol Plant

The use of supporting reference

One reference is found to acquire operating conditions as in the original reference. These specifications are listed in Table IV-2.

Table IV-2: Table of Carbonylation Reactor specification of Example by [21]

Reactor 114 specifications	Conditions/description	Page number
Temperature, C	175	5
Pressure, MPa	4 MPa	5
Catalyst active phase (metal)	Rhodium/Iodiude/triphenylphosphine	5
Catalyst Promoter	The iodine was initially employed as aquas hydiodic acid and in recycled form was present virtually entirely as methyl iodide	5
Solvent (component/composition)	In general, solvents are not required but they can present. Acetic acid and higher carboxylic acids, may fit.	2
Conversion/selectivity	Overall Methanol conversion of 64% Methanol selectivity to Methyl Acetate 65% Methanol Selectivity to Acetic Acid 35%	5
Other restrictions	-	-

According to the agreement between these specifications and the ones of original reference (Table above), this supporting reference can be used to obtain conversion/selectivity data.

By the end of presenting all alternative, the selection is made on the use of the reverse calculation method. The material balances conducted in the preceding subsections are used in order to complete the material balance with the methanol feed that is to be obtained by the conversion relation obtained from the supporting reference. Since the conversion is known by now, Methanol Feed can be calculated by the following relation from [27]:

$$x_A = \frac{Moles\ of\ A\ reacted}{Moles\ of\ A\ in\ the\ feed}$$

Since the amount unreacted is known (effluent of reactor, stream 134), then the moles reacted are simply the moles unreacted subtracted from the moles in the feed. By solver, the missing feed value is found. Pressure value that is used is 40 bar as an assumption within the recommended range. Mass balance, operating conditions, and stream data are available in Appendices B,C, and D respectively

Closing the Solvent Recycle loop

In principle, the solvent recycle represents a close loop, however, some of the amount is purged, while a new amount is added as a makeup, restricted by the composition calculated in the material balance. The significance of the former is to avoid expense of separation and/or avoid accumulation of contaminants. It is worth mentioning ere that closing the recycle loop is not equipped with a separate pump not a heater.

Section II Purification of Carbonylation product

The Carbonylation product obtained in previous unit is subjected for further processing. A first Methyl Acetate stream and an acetic acid streams are generated by separating the Carbonylation product stream, 136. [22] For simulation, the information needed to perform the separation by

distillation columns are the key components or what implies to them, compositions desired out of the separation for all components in the feed or at least the key components.

Because the components in the feed, stream 136, are ordered with increase in boiling point, considering relative volatility is the driving force because it is a distillation column, as the following: MeI, MeOAc, MeOH, H2O, Acetic Acid. Because the objective of this unit is to recover acetic acid and water in the lower part of the column, and MeOAc in the upper part, the key components are MeOAc and H2O. However, MeOAc has a lower boiling point than H2O and higher than MeOAc, it is specified and it is a reactant in the following unit, it was

They components are specified as MeOAC and AcOH not to represent the split between the key components based on boiling point, but rather to be able to specify component recovery since it is the target of this unit operation as per to the information mentioned in the Table above.

Basically, MeOAc recovery in top stream is specified as 98, while AcOH in the top stream to be 0.02. A higher recovery of MeOAc is specified in order to avoid exceeding the limits of mass concentration of MeI in the bottom stream. Note that acetic acid stream is taken from the bottom in the simulation as a bottom stream of heavy residue is not required because heavier by-products are not present and/or catalyst liquid were recovered in the preceding section of the plant. Otherwise, an extremely high recovery of MeOAc in the overhead stream is not necessarily required. No preconditioning is performed for temperature, while pressure brought back to 1 atm as a default option for atmospheric distillation, although not stated in the original reference.

Section III: Esterification of Acetic Acid and Methanol

The esterification unit is employed to produce Methyl Acetate, utilizing previously produced Acetic Acid from Carbonylation section. The esterification reaction involves the reaction of

esterifying an alcohol, that is converting an alcohol into an ester. For Ethanol production, Acetic Acid reacts with Methanol to produce Methyl Acetate as shown in the following reaction:

$$CH_3OH + CH_3COOH \rightarrow CH_3COOCH_3 + H_2O$$

This section of the plant consists of two main subsections: the reactor of where the esterification reaction takes place and the purification, of where the products get separated upon desire. In this work, a setup of reactor that is followed by a distillation column is employed. This setup is operated with selected operating conditions within the ranges mentioned as an approximation, and hence it shall be understood that this stands as an assumption. It is worth mentioning that a reactive distillation setup can be employed with the use of kinetics of the reaction as present in the work [28] and [29].

In this section, the acetic acid stream obtained from the bottom of previous column with water and is co-fed with Methanol to an esterification reactor. The following ranges, in Table IV-3, of operating conditions for the reactor are available by the original reference as per to the previously stated approximation of operating conditions.

Table IV-3: range specifications of esterification reactor by [22]

Reactor 120 specifications	Conditions/description	Page number
Temperature, C	100 to 150 100 to 130	15
Pressure, kPa	Atmospheric pressure. 50 to 500 50 to 400	15
Solvent (component/composition)	No use of a solvent is encountered within the text	-
Conversion/selectivity	High conversions of acetic acid to ester is preferred. For example, at least 80%, at least 90% or at least 95% of the acetic acid in acetic acid stream 142 is converted to an ester.	16
Feed ratio	the feed rates of acetic acid and methanol to the esterification unit 104 may be adjusted to control the mole ratio of acetic acid to methanol being fed to esterification unit 104. For example, the mole ratio of acetic acid to methanol fed to esterification unit 118 is from 1:1 to 1:15, e.g., from 1:1 to 1:5, or from 1:1 to 1:2	5 16

Section III Purification

The effluent of reactor is subjected to purification to recover MeOAc. Also other components are recovered for other purposes. To know the manner of how the technology presented in the original reference, careful reading of the text is conducted to properly identify the manner of purification. Since the reactor produces MeOAc, MeOH is fed in excess, conversion of

AcOH is less than 100%, water present in the feed and produced in the reaction, these four components are expected to appear in the reactor effluent. Additional to these component, other components may present on negligible quantities which flows from column 118 bottom stream along with purified AcOH with H_2O.

Section IV: Methyl Iodide removal

The first and second Methyl acetate streams are combined and fed to the methyl Iodide recovery unit. The reference [22] mentions benefits of removing alkyl halides such as Recycle to Carbonylation reactor. Methyl Iodide may be removed by one or more distillation columns. [22] In this work, one single column could accomplish the task. Because DSTWU is unable to calculate the minimum reflux ratio, a RadFrac model is directly installed with an initial guess until stat factory results are obtained.

Section V: Hydrogenolysis of Methyl Acetate

In this section, Hydrogen is reacted with the previously produced Methyl Acetate to give Ethanol and co-produce methanol. This conversion is obtained via the Hydrogenolysis reactions as follows:

$$H_2 + CH_3COOCH_3 \rightarrow CH_3CH_2OH + CH_3OH$$

In general, for Ethanol plant presented in the original reference [22], the following ranges are recommended for Hydrogenolysis reactor operating conditions.

Table IV-4: ranges of preferred operating conditions of Hydrogenolysis reactor by [22]

Reactor specifications	Conditions/description	Page number
Temperature, C	125° C. to 350° C 180° C to 345° C 225° C to 310°C	18
Pressure, kPa	greater than 3,000 kPa greater than 5,000 kPa. from 700 to 8,500 kPa from 1,500 to 7,000 kPa, from 2,000 to 6,500 kPa. greater than 2,500 kPa	18
Solvent (component/composition)	not encountered	
Conversion/selectivity	at least 75% at least 85% at least 90% at least 95% at least 97%	12
Feed ratio	molar ratio of hydrogen to methyl acetate is greater than 10:1, e.g., greater than 15:1, or greater than 20:1.	18

In this work, as an approximation, the reactor runs at 40 bar and 473 k with an approximated conversion of 95%, and hence it shall be understood that these operating conditions

that are selected from the ranges available in TableIV-4 stand as assumptions. For more precise operating conditions, experimental data may be found in [30].

By simulating the Hydrogenolysis section, the overall plant simulation flowsheet is completed. Figure IV-10 shows an overall view. Mass balance, operating conditions, and stream data are available in Appendices B,C, and D respectively

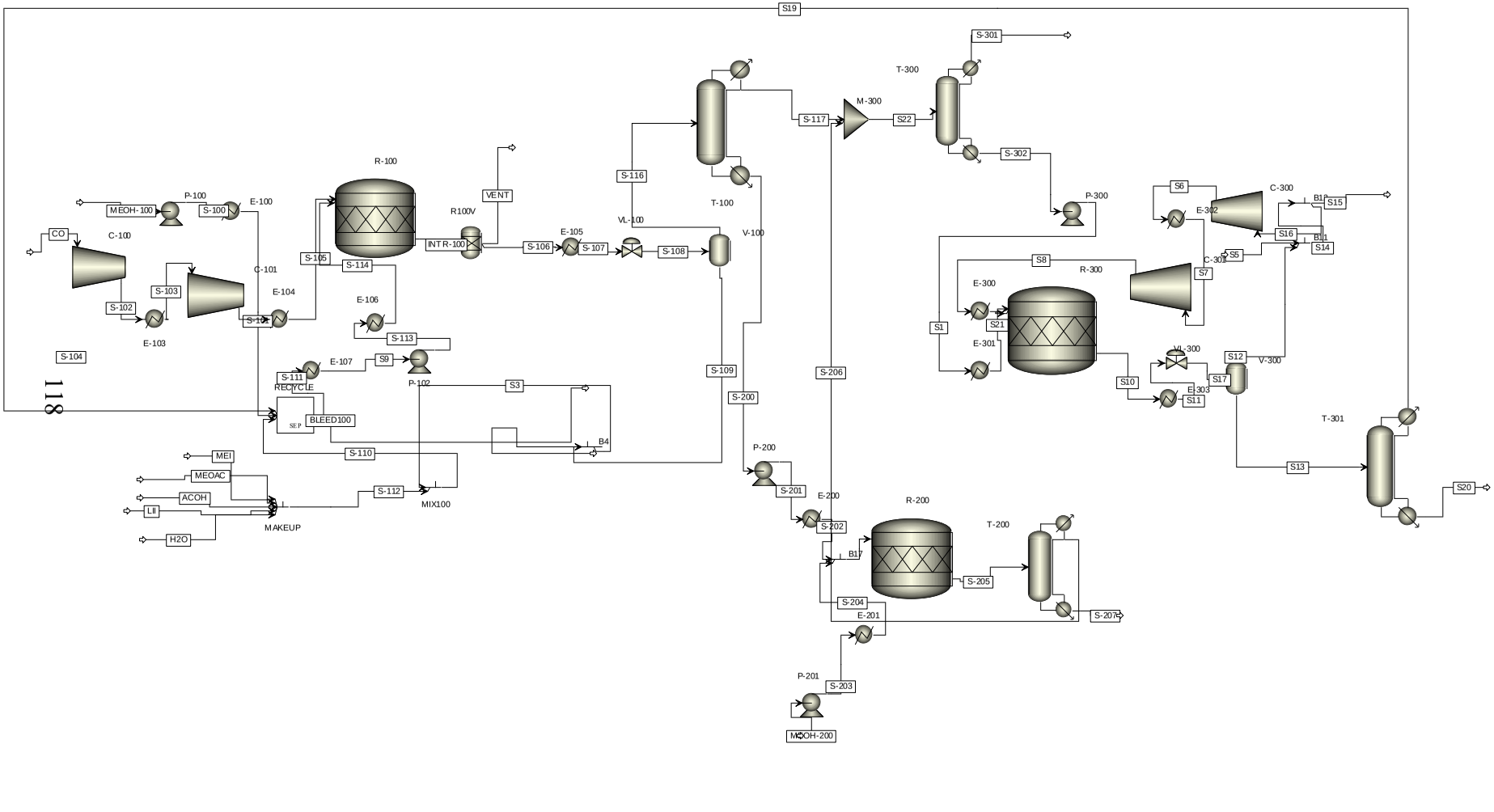

Figure IV-10: Simulation Environment of Ethanol Plant by using Aspen Plus ™

IV.5 STAND-ALONE PLANTS: HEAT INTEGRATION

The thermodynamic feasibility to match heating and cooling targets in a chemical process may be achieved by pinch analysis via heat integration. In principle, heat integration is an approach to minimize the use of utilities needed for cooling and heating as addressed earlier in details in this work. As illustrated since the very beginning of this work, heat integration represents a basic phase of plant design. It represents the layer of heat recovery. In order for heat integration to be done, an energy balance of the given process is needed. By the energy balance, the types of the utilities that is to be used for the system can be determined. In this work, the utilities suggested by Aspen Plus™ are taken into consideration. Heat integration is performed in a given chemical plant after all material balance and energy balances are performed. This information represents the important starting point to integrate the heat sources and sinks in a given chemical plant.

- Data extraction:

  For data extraction, the original non-heat integrated flow sheet needs to be prepared. The extraction of information from a flowsheet with many constraints may result in loss of the integration opportunities. [8] The data extraction has the following considerations:

a. Limiting heat exchanger segments to one. This one heat exchanger represents the initial and final desired temperature values of a process stream. This is done in order to minimize un-needed constraints as justified earlier in this text.
b. The distillation columns do not participate in heat exchanger network (HEN). This action is taken because the application of distillation column for matching streams an d exchanging stream could not be found in a dedicated model in Aspen Plus TM such as MHeatX etc.

c. For the coolers and heaters of reactors. They were not simulated prior to data extraction to avoid an expected conflict since it is supposed that Aspen Plus™ accounts for it by default. Yet, in this research, an attempt is made to simulate the generation of steam from the reactor evolved heat. generated stream in case the streams of steam generation are used for data extraction for the generation of HEN. For Low pressure steam generation, for example, boiler feed water saturated at 124 C that eventually utilizes the excess hear from the reactor to generate LP Steam as a feature of the reactor setup. Also, this action is taken after an attempt to heat-integrate the flowsheet without the addition of the cooling setup of the reactor (in order to increase integration opportunities by minimizing constraints) which eventually resulted in setting up a LP Steam generation as the cold side stream. Taking one reactor as an example, the reaction of Carbonylation is exothermic. It generates heat.

Aspen Energy Analysis specifies Low pressure steam generation from the heat of the reaction. It mentions that the cold stream (steam) enters at 124 °C and leaves as LP Steam at 125 °C. Thus the following procedure is followed to setup the heat exchanger of LP Steam generation from the Carbonylation reactor:

1. The model Heater is used

2. water stream enters the cold side

3. A heat stream is installed out of the reactor and enters the heater.

5. The inlet cold stream specifies temperature at 124 °C and vapor fraction of 0 (saturated liquid)

6. The heater outlet temperature is specified as 125 °C.

7. The inlet flow rate of water affects the phase status in the outlet. For example, if very high flow rate is specified, the heat is not sufficient to vaporize it to saturated

vapor, and vice versa. Tus a trial and error approach is followed until the vapor fraction at the outlet is 0

8. Additional to point 7, in order to make sure that a superheated is generated but saturated vapor, the saturation pressure of steam at 125 C is calculated as shown in the following table. Once the outlet stream has this pressure for a given flowrate, then the setup is satisfied. The yellow cells in the table below are obtained by linear interpolation.

Table IV-5: Evaluating saturated vapor water at 125 C, data by Ref. [31]

Pressure, bar	Pressure, kPa	Temperature, °C
2.25	225	123.97
2.324855	232.4855	125

9. For this setup, a thermodynamic model STEAM-TA is used under flowsheet section.

d. Number of designs were generated per plant; the selection of a heat integrated network design took into consideration the following:

- The main selection priority is given to HEN that has the minimum integration of reactor heat streams and process streams. This is because of the technical limitations in applying the respective heat exchanger. This limitation is represented in sizing the heat exchanger that accepts a heat stream as mentioned earlier.

- The overall Capital and Utility cost should not deviate significantly from the least expensive HEN design available
- The maximum split branches for every heat exchanger is specified to be 1 to minimize complications and computational efforts.

e. Consideration/assumptions of Simulation of the heat Exchanger Network (upgrading the simulated flowsheet of the plant with the HEN)

1. When two heat exchangers from sections that are simulated with different thermodynamic packages, priority is given to NRTL-HOC package over SR-POLAR. This is because the presence of Acetic Acid is, by the experience of the author of this work, has a more dominating effect, than the high pressure for pressures above 15 atm, since the latter is in either way being estimated.
2. Assumption mentioned in point 1 is applied unless an explicit error is encountered by the simulation software for exceeding the pressure limit.
3. It shall be understood that a full commitment of application of assumption mentioned in point 1 since it may happen that a heat exchanger is installed in another section without intention. In this case, it is assumed that the effected is minor since SR-POLAR uses Wilson activity coefficient model as stated earlier which hold for non-ideality in liquid state, and uses UNIFAC or HOC for the gas phase, hopefully parameters in HOC were selected by the simulation software.
4. MHeatX model is used to represent heat exchangers for matching process-process streams
5. Heater Model is used to represent heat exchangers for matching process-utility streams

6. For heat exchangers that match process-utility streams, the utility in principle, although known, is not specified since sometimes it may result in a consistency error. In this case, Aspen Plus will by default assign a utility type for the given heat exchanger.
7. For heat exchangers that match process-process streams, the temperature specification (that has a constraint of having at least one stream un-specified) priority id given for the stream that approaches its final destination temperature-value. Otherwise, the specification is followed for one stream for a series of heat exchangers.
8. The significance of the previous point: when HEN is applied on the flowsheet, the exact temperature values of the original HEN design may not be as exact when applied to the Aspen Plus process flowsheet, generating possible errors and/or warnings.
9. The pressure specification is kept as for pressure drop. The pressure drop specification follows heuristics as stated earlier in the simulation phase.
10. Exception on point 7 takes into account manipulating the pressure drop value in case the heat exchanger does not converge/being sized/wrongly calculates the desired temperature outputs. This modification is kept, roughly, around the value recommended by heuristics for the respective phase.
11. Continuing from the previous point, the phase of the inlet and outlet fluids change after generating the HEN. Thus, an initial estimation of the phase change according the knowledge about the fluid phase behavior is specified, then, after the HEN is

well established in the design of the plant, s re-specified the pressure drop specification is re-specified.

IV.5.1.1 Plant I (Acetic Acid Production by Methanol Carbonylation)

At Acetic acid plant, there are total of five heat exchangers, excluding distillation column. One recommended design by Aspen energy analyzer is summarized in Tables F-1 and F-2 in Appendix F. These tables include information about stream matching in the selected network for Acetic Acid plant along with their temperature segments. These data are used to apply the network design on the simulation environment of Acetic Acid standalone plant. The overall simulation environment of Acetic Acid standalone plant that is loaded with the selected heat exchanger network is shown in Figure IV-11. It is worth mentioning that Figure IV-11 is the reference simulation flowsheet for the coming sections as well as for the tabulated data in the Appendices since the heat integration step wraps up the plant design phase with respect to plant flowsheet.

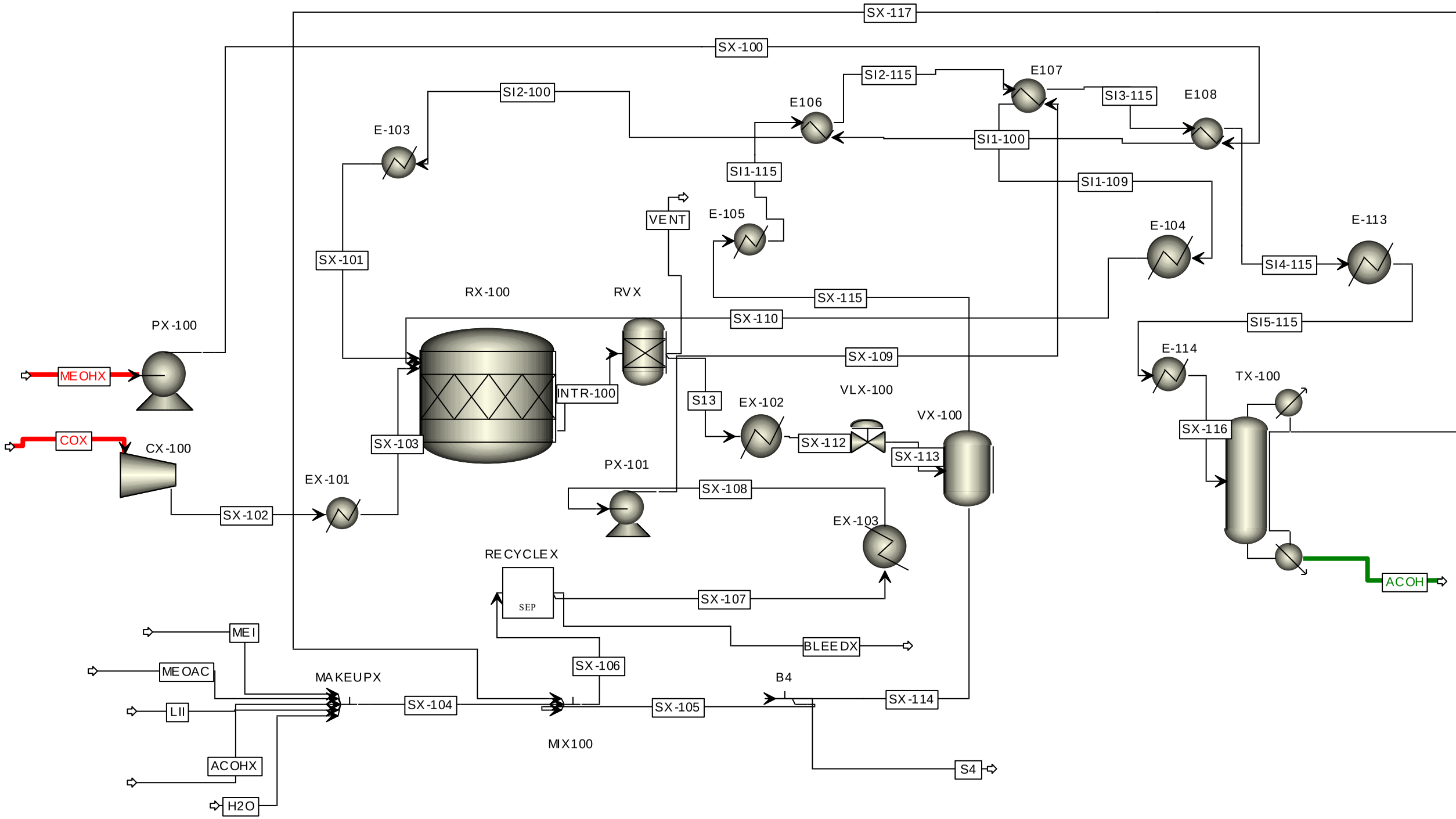

Figure IV-11: Acetic Acid Standalone Plant with Heat Integration Network Flowsheet in Aspen Plus™ Simulation Environment

The utility system of cooling and heating after heat integration is affected. One way to assess the performance of the applied heat integration network is to review the utility systems of the Acetic Acid plant before and after heat integration. Tables IV-6 and IV-7.

Table IV-6: Utilities System of Acetic Acid Standalone Plant before Heat Integration

	Current	**Target**	**Energy Cost Savings**	**Energy Cost Savings**	**ΔTmin**	**Status**
	[cal/sec]	**[cal/sec]**	**[$/Yr]**	**[%]**	**[C]**	
LP Steam	4814	0	1,208	100	10	
HP Steam	2.14E+06	7.06E+05	473,777	67.01	10	
Total Hot Utilities	2.15E+06	7.06E+05	474,986	67.07		Sufficient
LP Steam Generation	5.68E+06	5.00E+06	-168,318	-11.88	10	
Air	1.73E+06	9.69E+05	101	44.13	10	
Total Cold Utilities	7.41E+06	5.97E+06	-168,217	-11.87		Sufficient

Table IV-7: Utilities System of Acetic Acid Standalone Plant After Heat Integration

	Current	**Target**	**Energy Cost Savings**	**Energy Cost Savings**	**ΔTmin**	**Status**
	[cal/sec]	**[cal/sec]**	**[$/Yr]**	**[%]**	**[C]**	
U-2	2.04E+06	7.11E+05	440,132	65.22	10	
Total Hot Utilities	2.04E+06	7.11E+05	440,132	65.22		Sufficient
U-1	7.31E+06	5.97E+06	0	0	10	
Total Cold Utilities	7.31E+06	5.97E+06	0	18.24		Sufficient

Because heat integration does not have an effect on utilities system only, but also capital cost, an assessment of this effect is analyzed. The effect on Capital cost takes place due to the change in the heat exchanger in terms of number and temperature difference which does affect the area of the equipment. These changes are responsible for the change in capital cost. Table IV-9 shows the effect on major cost parameters at Acetic Acid Plant.

Table IV-8: Summary of Acetic Acid Plant Performance influenced by Heat Integration

Name	Before Heat Integration	After Heat Integration	Percentage	Effect
Total Capital Cost [USD]	11786800	14916000	26.5%	Increase
Fixed Cost* [USD/Year]	2664180	2637870	1.0%	Decrease
Total Utilities Cost [USD/Year]	6335300	5806710	8.3%	Decrease
Equipment Cost [USD]	2433200	3382100	39.0%	Increase
Total Installed Cost [USD]	4527100	6171600	36.3%	Increase

*Fixed cost is calculated as Operating Cost-Utilities cost as defined by Aspen Plus™ V.8.1

It can be observed that the capital cost, equipment cost, and total installed cost have a negative effect as they increased after heat integration. However, the heat integration benefited the plant by decreasing the fixed cost and utility cost.

IV.5.1.2 Plant II (Ethanol Production from Methyl Acetate)

One HEN design scenario is selected from over 50 designs with satisfactory overall utility and economic performance. The generated heat exchanger network is classified in tables, showing the stream connections. This network is applied on Aspen Plus flowsheet file, and total savings are later illustrated. The heat exchanger design network that is used for Ethanol Plant can be found in Tables F-1 through F-3 in Appendix F of where all needed design parameter to apply the network are available. As in the Acetic Acid plant section, the influence of Heat Integration on the utilities system is emulated. The data related to utilities system of Ethanol plant before and after heat integration are available in Tables IV-9 and IV-10 respectively. Note that for some utilities, the use is increased while it is being decreased for other utilities, giving an overall positive effect on the utility cost. This utility cost along with other cost parameters are evaluated, showing the effect of heat integration by comparing the plant before and after Heat Integration as shown in Table IV-11 which represents the reference to the tabulated data in the Appendices since the heat integration step wraps up the plant design phase with respect to plant flowsheet.

Table IV-9: Utility System of Ethanol Plant before Heat Integration

	Current	Target	Energy Cost Savings	Energy Cost Savings	ΔTmin
	[cal/sec]	[cal/sec]	[$/Yr]	[%]	[C]
HP Steam	3.42E+06	4.10E+05	995,645	88.04	10
LP Steam	6.26E+06	3.81E+06	614,903	39.13	10
MP Steam	1.26E+06	1.27E+05	327,933	89.88	10
Total Hot Utilities	1.09E+07	4.35E+06	1,938,480	63.2	
Cooling Water	1.15E+06	1.56E+05	27,758	86.37	5
Air	6.82E+06	8.01E+06	-158	-17.48	10
LP Steam Generation	3.42E+06	0	-854,299	-100	10
MP Steam Generation	1.03E+05	0	-29,923	-100	10
Refrigerant 1	3.61E+06	3.36E+05	1,183,535	90.68	3
Total Cold Utilities	1.51E+07	8.50E+06	326,914	72.02	

Table IV-10: Utility System of Ethanol Plant after Heat Integration

	Current	**Target**	**Energy Cost Savings**	**Energy Cost Savings**	**ΔTmin**
	[cal/sec]	**[cal/sec]**	**[$/Yr]**	**[%]**	**[C]**
HP Steam	2.01E+06	6.14E+05	462,382	69.52	10
LP Steam	9.17E+05	0	230,085	100	10
MP Steam	8.01E+05	1.48E+05	189,767	81.55	10
Total Hot Utilities	3.73E+06	7.62E+05	882,234	78.22	
Air	3.14E+06	3.58E+06	-58	-14.1	10
LP Steam Generation	3.42E+06	7.73E+05	-661,268	-77.4	10
MP Steam Generation	1.15E+05	0	-33,238	-100	10
Refrigerant 1	1.09E+06	4.42E+05	234,820	59.51	3
Total Cold Utilities	7.77E+06	4.80E+06	-459,745	-93.35	

Table IV-11: Summary of Ethanol Plant Performance influenced by Heat Integration

Name	Before Heat Integration	After Heat Integration	Percentage	Effect
Total Capital Cost [USD]	32230500	34583100	7.3%	Increase
Fixed Cost* [USD/Year]	5073100	4852300	4.4%	Decrease
Total Utilities Cost [USD/Year]	18140600	15292100	15.7%	Decrease
Equipment Cost [USD]	8827000	9321100	5.6%	Increase
Total Installed Cost [USD]	14376300	15492400	7.8%	Increase

*Fixed cost is calculated as Operating Cost-Utilities cost as defined by Aspen Plus™ V.8.1

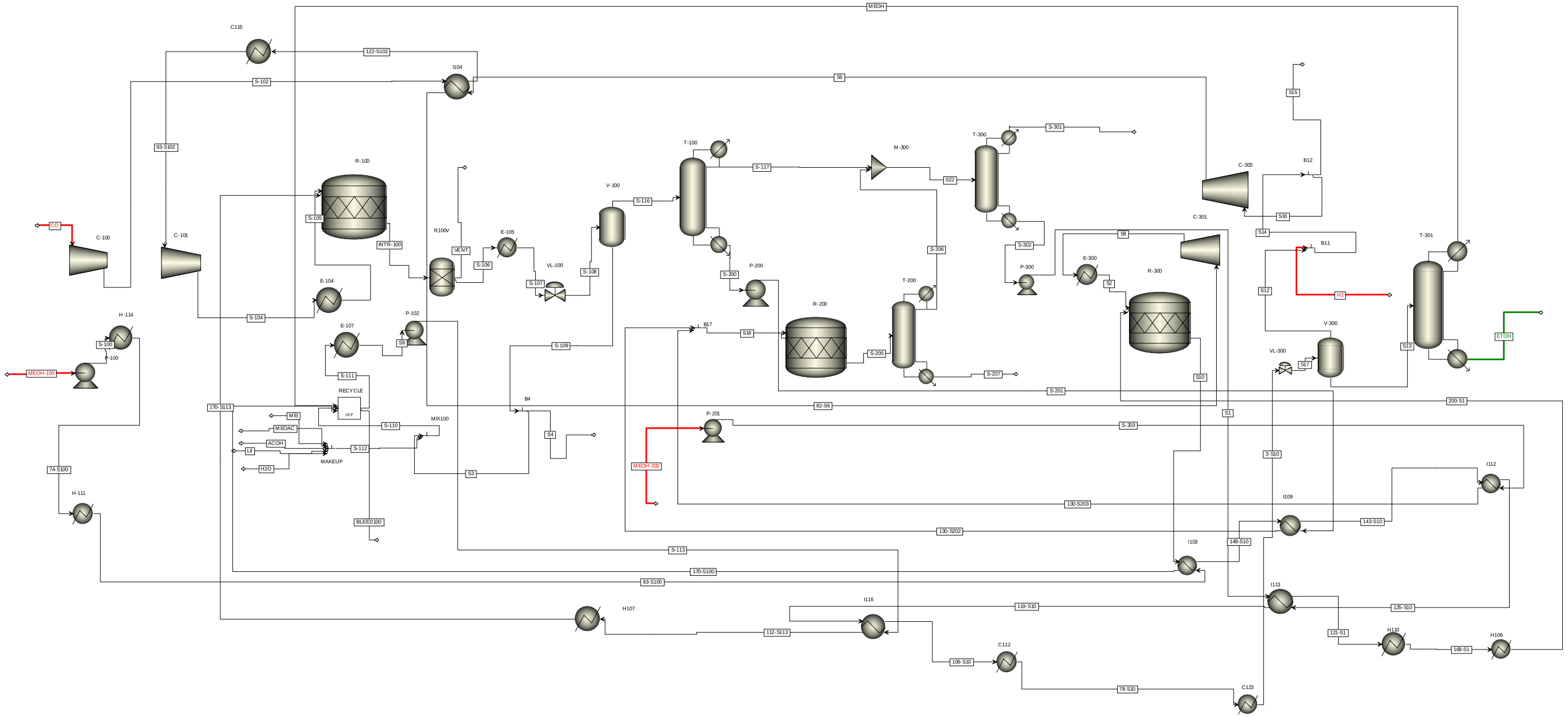

Figure IV-12: Ethanol Standalone Plant with Heat Integration Network Flowsheet in Aspen Plus^{TM} Simulation Environment

IV.6 STAND-ALONE PLANTS: ECONOMIC EVALUATION

The ultimate goal of investing in a chemical industry is making a profit. A given chemical plant should be economically justified in order to invest on it. Main factors that affect the economics of a chemical plant are Capital cost, operating cost, utility cost, raw material cost, and product demand or product price. These factors define the money flow from and to a chemical plant. In order to analyze the economic performance of the stand-alone plants in this study, the amount of raw material is obtained as the following:

Table IV-12: Raw Material and Product Prices

Chemical	Value	Unit	Price/mass, $/tonne	Reference
CO	70	$/Ton	70	[32]
H2	0.135	$/m3		[32]
Ethanol 99%	850	GBP/tonne	1,168.74	[33]
Ethanol 96%	72	EUR/Ton	89.38008	[33]
Methanol	445	EUR/Ton	542.557	[33]
Acetic Acid	725	$/MT	725	[33]

Table IV-13: Raw material amounts in the two stand-alone plants

	Acetic Acid Plant	Ethanol Plant
Fresh Feed		
Hydrogen approximate, m3/year	-	64,820,145.60
Carbon Monoxide, Ton/year	182,058.82	198,988.47
Methanol, Ton/year*	179,629.06	127,857.05
Product		
Ethanol, Ton/year	-	128,107.20
Acetic Acid, Ton/year	333,685.25	-

*Methanol amount is calculated as the net Methanol in the plant. This assumes that all produced

Methanol by Ethanol plant is assumed to be recycled. It cannot be included in sales because the grade is relatively low to be a salable finished product. This assumption disregards the purity of the recycle.

Because accounting for the product price, huge difference is obtained in profitability when comparing a scenario of accounting for Ethanol of grade 96% with the one of 99%. In this study, Ethanol is 97%, and making a comparison might be not wise decision based on the given information. Thus, the analysis of the economic performance in this context is limited to the Annualized cost. The following table represents the prices of raw material of every plant:

Table IV-14: prices of raw material used in the two stand-alone plants

	Acetic Acid Plant	Ethanol Plant
Hydrogen approximate, $/year	-	8,750,719.66
Carbon Monoxide, $/year	12,744,117.18	13,929,193.05
Methanol, $/year	97,459,001.74	69,369,739.13

The annualized cost follows the procedure of annualizing the capital cost by dividing into the plant life period. The total costs in the unit of price/time are added. Table IV-15 shows the economics/cost parameters for both standalone plants.

Table IV-15: Stand-alone plants Annualized Capital Cost

	Ethanol Plant	Acetic Acid Plant
Capital Annualized Cost*	3.45E+06	1.49E+06
Utilities Cost	1.53E+07	5.81E+06
Fixed Cost**	4.85E+06	2.64E+06
Total Annualized Cost	2.36E+07	9.94E+06

*Based on Project Life =10 years

**Fixed cost is calculated as Operating Cost-Utilities cost as defined by Aspen Plus™ V.8.1

According to costs calculations, on annual bases, the two plants costs are on a similar level.

The other parameters and specifications of economic analysis and evaluation can be found in Appendices E.1 and E.2 for Acetic Acid and Ethanol plants respectively.

CHAPTER V

ILLUSTRATIVE EXAMPLE PART II: APPLICATION OF STRUCTURAL INTEGRATION APPROACH

The use of the algorithm requires minimum information about the technology of the process flow diagram elements (equipment), the function of the equipment and the flow of components among its streams. This information represents essential input for the Matrix generation which is the key step to initiate any of the developed algorithms. As a general guide, the more realistic the flows and process flow diagram used as an input, the more the realistic are the generated opportunities.

V.1 ENCODED PROCESS FLOW DIAGRAMS OF THE STANDALONE PLANTS

In order to use the systematic approach that is developed towards structure integration, the original process flow diagrams need to be encoded. First, the flow of elements around the units of interest within the process flowsheet units needs to be identified and highlighted to make the translation to the encoded flow diagram easier. Figure V-1 shows the process flow diagram of Acetic Acid Plant simulated in this work embedded with the flow of components around the distillation column and the reactor. Note that the inert/solvents are not included in defining the reactor boundaries. This is because they do not participate in the chemical reactions of the given reactor. In order to minimize text, the encoding of selective units is described and First, each element is given a number to be presented in a row, defining the C dimension. Thus, Acetic Acid (AcOH)=1, Water (H2O) =2, MeOAc (Methyl Acetate)=3, Methanol (MeOH)=4, CO (Carbon Monoxide)=5, Methyl Iodide (MeI)=6, Ethanol (EtOH)=7, and Lithium Iodide (LiI)=8. The encoded process flow diagram of Acetic Acid plant is represented in Figure V-2. The following description maybe useful to illustrated how the encoding is performed:

Encoding the Carbonylation reactor:

- CO is encoded as -2 because it is a reactant that is fed in excess.
- MeOH is encoded as -1 because it is a limiting reactant
- AcOH is encoded as 1 since it is a main-process product

Encoding the distillation column of Acetic Acid Plant

- AcOH is encoded as 1 since it is being separated as a heavy key
- The other component is encoded with negative sign in increasing magnitude with decreasing boiling point. The light key is water and it is given a value of -1

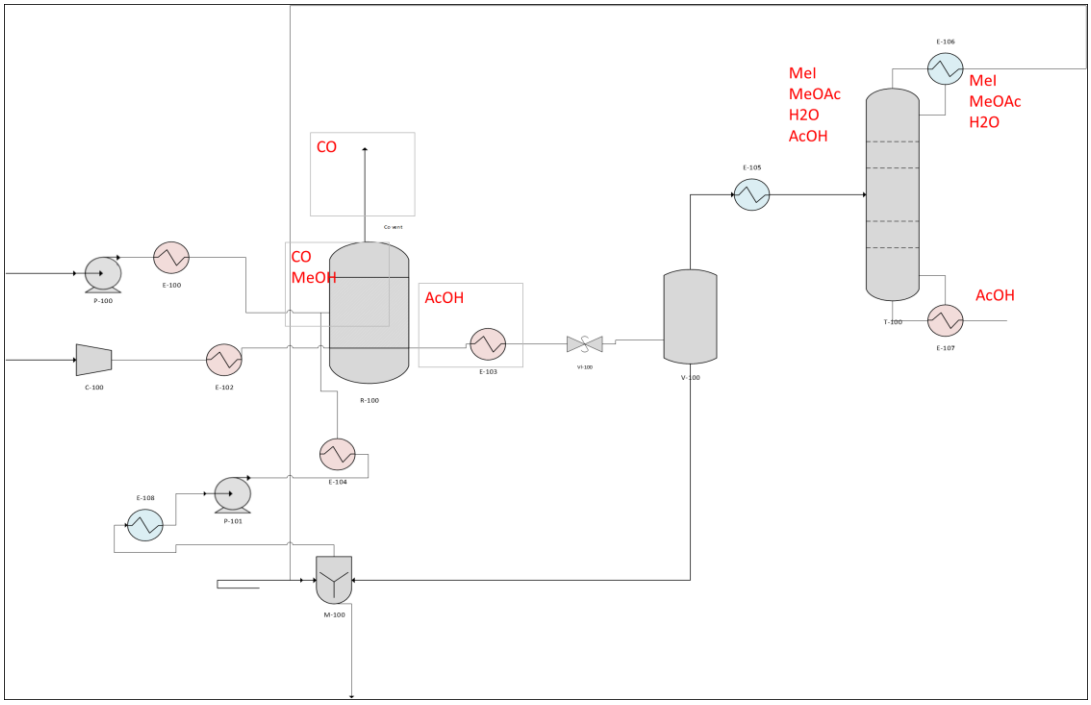

Figure V-1: Acetic Acid process flow diagram with the flow of chemical species.

Encoded Acetic Acid Plant		
	1 (column)	2 (reactor)
AcOH	1	1
H2O	-1	0
MeOAc	-3	0
MeOH	-2	-1
CO	0	-2
H2	0	0
MeI	-4	0
EtOH	0	0
LiI	0	0

Figure V-2: Encoded Acetic Acid Plant

Ethanol process flow diagram is shown in Figure V-3 loaded with the flow of components around the operating units. This flow diagram is encoded as shown in Figure V-4. The following points provide description of how selective units of which encoding other units followed same manner.

Encoding MeI Recovery Unit

- MeI is encoded as -1 because it is the light key component.
- MeOH is encoded as 21 because it is being distributed among the light and heavy cuts. Although the mass fraction is distributed almost equally it is encoded as 12, tending more to the heavy cut because the basic intention behind implementing the MeI recovery unit is to recover MeI as the name indicates.
- MeOAc is encoded as -1 since it is the heavy key.

Encoding the Carbonylation reactor:

- CO is encoded as -2 because it is a reactant that is fed in excess.
- MeOH is encoded as -1 because it is a limiting reactant
- MeOAc is encoded as 2 since it is a main-reactor product
- AcOH is encoded as 5 since it is a side product (thus it is given the first available positive integer from the range 5 to infinity)

Encoding the esterification reactor:

- MeOH is encoded as -2 because it is a reactant that is fed in excess.
- AcOH is encoded as -5 because it is a reactant that comes from a process stream and holds the condition of being a side product. Thus, the coefficient that it had as a side produced is encoded here with a negative sign because it is being consumed in this reactor.
- MeOAc is encoded as 2 since it is a main-reactor product
- H2O is encoded as 6 since it is a side product (thus it is given the second available positive integer from the range 5 to infinity)

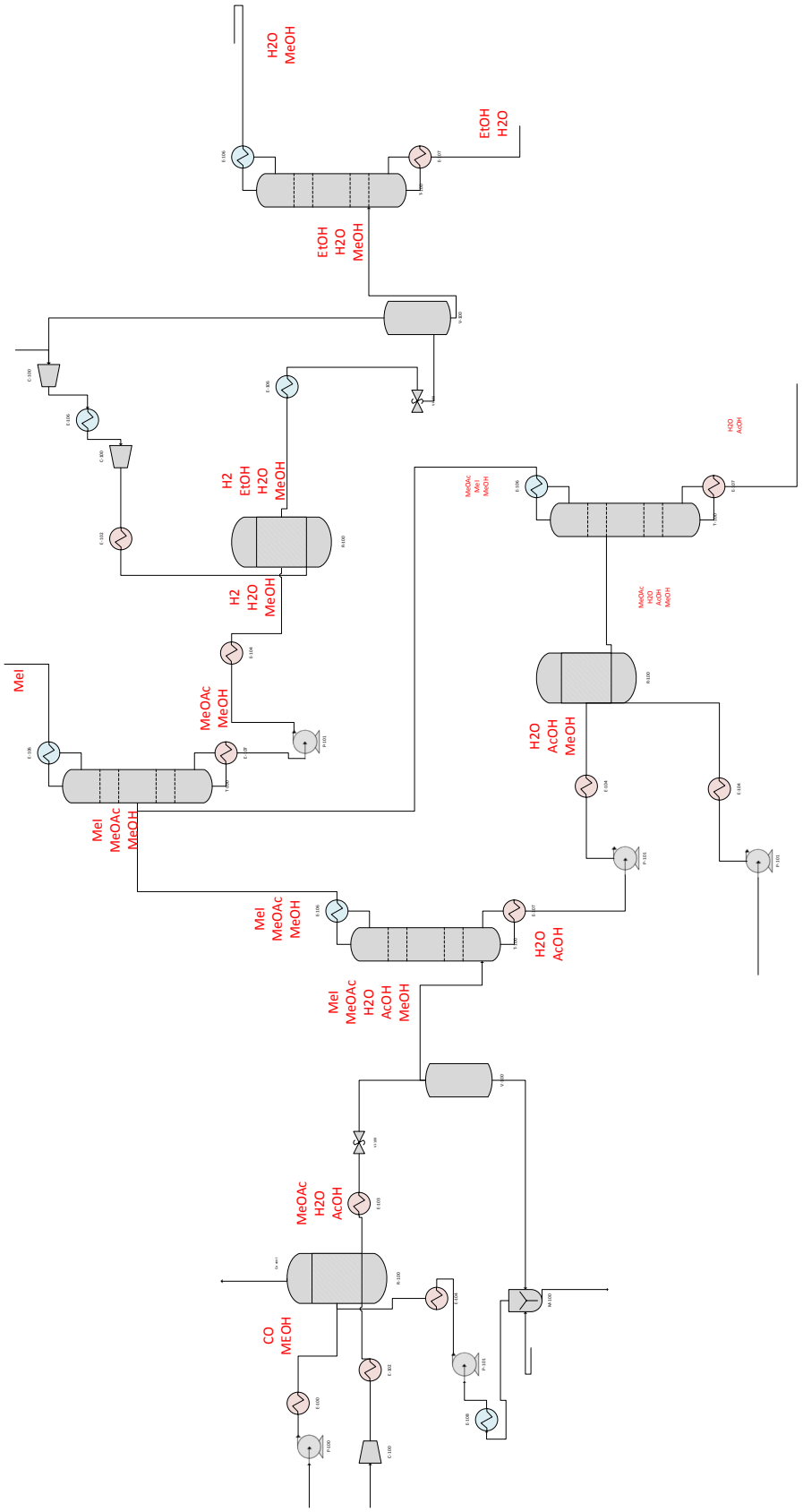

Figure V-3: Ethanol plant process flow diagram loaded with the flow of chemical species.

Encoded Ethanol Plant							
	1 (column)	2 (reactor)	3 (column)	4 (reactor)	5 (column)	6 (reactor)	7 (column)
AcOH	2	5	2	-5	0	0	0
H2O	1	0	1	6	0	0	21
MeOAc	-2	2	-1	2	1	-1	0
MeOH	-1	-1	12	-2	21	2	-1
CO	0	-2	0	0	0	0	0
H2	0	0	0	0	0	-2	0
MeI	-3	0	0	0	-1	0	0
EtOH	0	0	0	0	0	1	1
LiI	0	0	0	0	0	0	0

Figure V-4: Encoded Ethanol Plant

V.2 APPLICATION OF DEVELOPED ALGORITHM FLOWSHEETS

The encoded flowsheets are subjected to the reactor algorithm flowchart. The flowchart starts by evaluating row by row in identifying similar chemical species. Hereby, as shown in Figure 9.5, evaluation of row n=1 results in identification of a common element as highlighted as shown in Figure 9.3. This element is Acetic Acid. It does exist in the first reactor (at column 2 of matrix 1) with a coefficient of 5, indicating a side production of Acetic Acid. In the other plant, it does exist with a coefficient of one, indicating the production of a main-process product. By following the steps as shown in Figures 9.7 and 9.8, Acetic Acid plant can be donated to as original P element. Then, at step 32, a question about the existence of the element at the other plants for following reactors is addressed. In this case, at column 4, that is the second reactor in the process, Acetic Acid is identified. Then, by following the next steps, the flowchart checks the attribution to eventually find out that it is being consumed, making up the case of utilization of a side product. A further check about the coefficient magnitude assures the previously stated information. Then at step 40, a question about other components in the later reactor is addressed in order to assure about whether it is being consumed to produce a component that exist originally in the former reactor. When this case is satisfied, a synergy type is figured out: there is synergetic opportunity of partially/fully similar operations/reactions.

Then, the algorithm flowchart takes further routes to check over the other rows. This results in identifying another common element across plants as shown in Figure V-5. The application of the approach is shown in Figures V-5 and V-6. This row is row n=3 of which the element that is identified is Methanol. As shown in the steps of running the algorithm flowchart at Figures V-7, V-8, V-9, and V-10, the system reach to step 14 to find out that all identified elements hold negative sign. Then, when the row is subjected to the loop that starts with step 59, it eventually

identified that there is no component that exist as a reactant while being consumed in the other plant for the given reactors of where the originally identified element exist. Then, the system passes though the loop that starts with step 63 that is being terminated when the system detects that not all elements in the respective reactors across plants are actually the same. Then, the system is by-passed to step 68 to check whether the previous result from step 63 is a result from differences of the feed, product, or both. Eventually, it detects that the feed stock is identical and figures out a synergy type of identical feed stock. Then the system goes through route A to check the elements that may be partially similar, to find them out with encoded symbol as Yi. Hereby, a detection of partially similar production exists.

	Ethanol Plant						
	1 (column)	2 (reactor)	3 (column)	4 (reactor)	5 (column)	6 (reactor)	7 (column)
AcOH	2	**5**	2	-5	0	0	0
H2O	1	0	1	6	0	0	21
MeOAc	-2	2	-1	2	1	-1	0
MeOH	-1	-1	12	-2	21	2	-1
CO	0	-2	0	0	0	0	0
H2	0	0	0	0	0	-2	0
MeI	-3	0	0	0	-1	0	0
EtOH	0	0	0	0	0	1	1
LiI	0	0	0	0	0	0	0

	Acetic Acid Plant	
	1 (column)	2 (reactor)
AcOH	1	**1**
H2O	-1	0
MeOAc	-3	0
MeOH	-2	-1
CO	0	-2
H2	0	0
MeI	-4	0
EtOH	0	0
LiI	0	0

	Ethanol Plant						
	1 (column)	2 (reactor)	3 (column)	4 (reactor)	5 (column)	6 (reactor)	7 (column)
AcOH	2	**5**	2	-5	0	0	0
H2O	1	0	1	6	0	0	21
MeOAc	-2	**2**	-1	**2**	1	-1	0
MeOH	-1	-1	12	-2	21	2	-1
CO	0	-2	0	0	0	0	0
H2	0	0	0	0	0	-2	0
MeI	-3	0	0	0	-1	0	0
EtOH	0	0	0	0	0	1	1
LiI	0	0	0	0	0	0	0

	Acetic Acid Plant	
	1 (column)	2 (reactor)
AcOH	1	**1**
H2O	-1	0
MeOAc	-3	0
MeOH	-2	-1
CO	0	-2
H2	0	0
MeI	-4	0
EtOH	0	0
LiI	0	0

Figure V-5: Application of Reactor Algorithm flowchart to the case study part 1

Encoded Ethanol Plant							
	1 (column)	2 (reactor)	3 (column)	4 (reactor)	5 (column)	6 (reactor)	7 (column)
AcOH	2	5	2	-5	0	0	0
H2O	1	0	1	6	0	0	21
MeOAc	-2	2	-1	2	1	-1	0
MeOH	-1	**-1**	12	-2	21	2	-1
CO	0	-2	0	0	0	0	0
H2	0	0	0	0	0	-2	0
MeI	-3	0	0	0	-1	0	0
EtOH	0	0	0	0	0	1	1
LiI	0	0	0	0	0	0	0

Encoded Acetic Acid Plant		
	1 (column)	2 (reactor)
AcOH	1	1
H2O	-1	0
MeOAc	-3	0
MeOH	**-2**	-1
CO	0	-2
H2	0	0
MeI	-4	0
EtOH	0	0
LiI	0	0

Figure V-6: Application of Reactor Algorithm Flowchart to the case study part 2

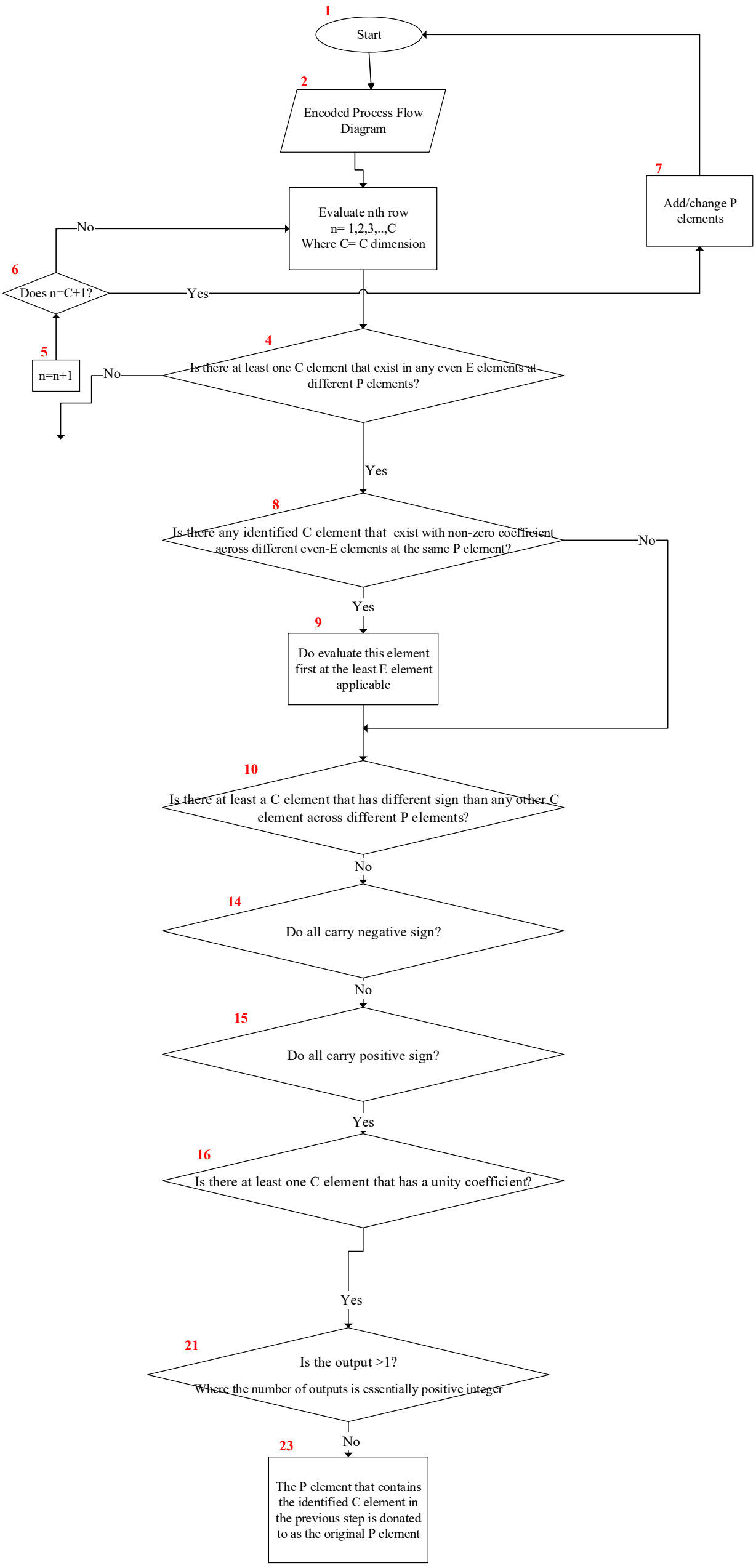

Figure V-7: Flowchart steps applied for part 1, a

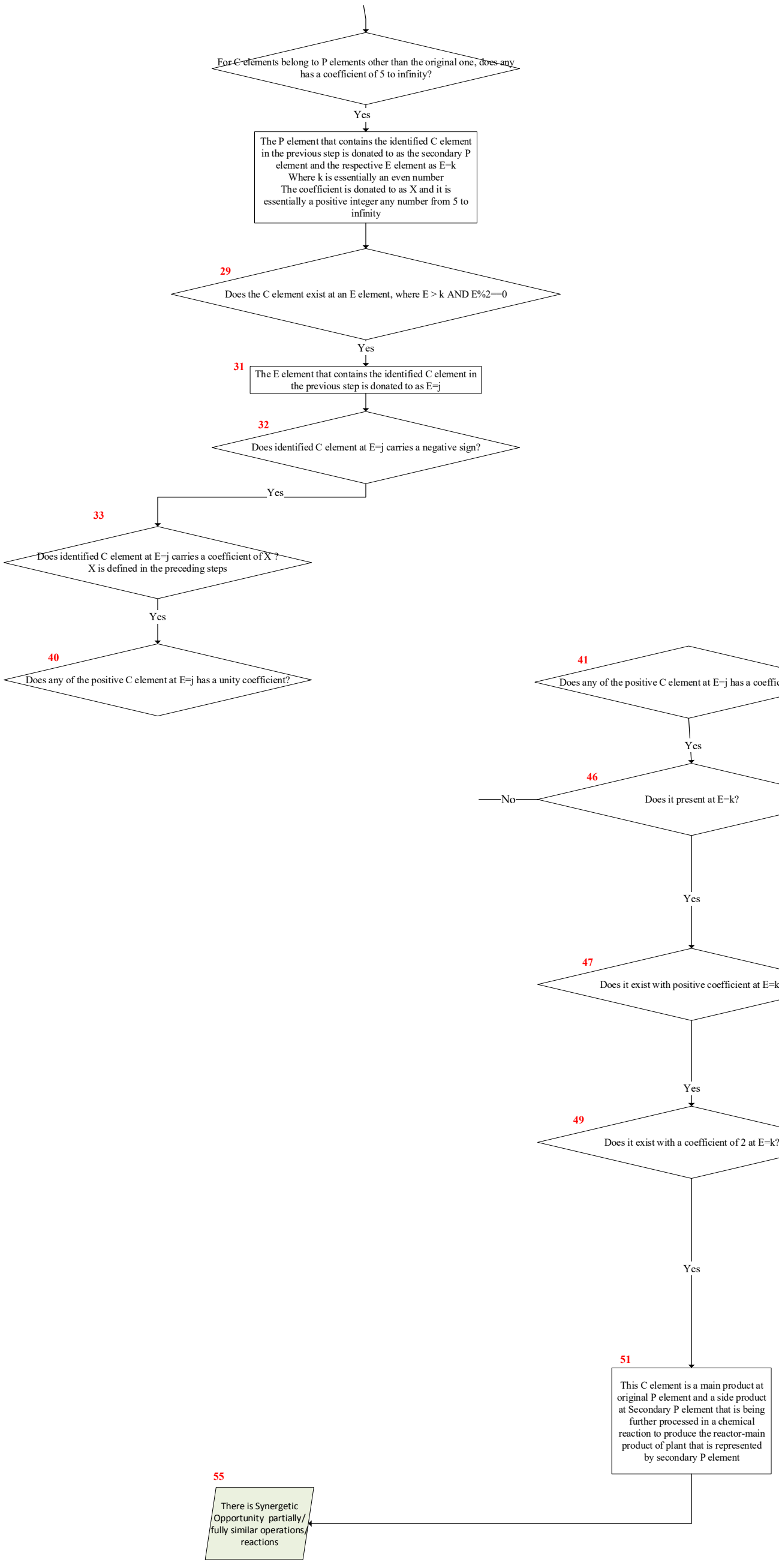

Figure V-8: Flowchart steps applied for part 1,b

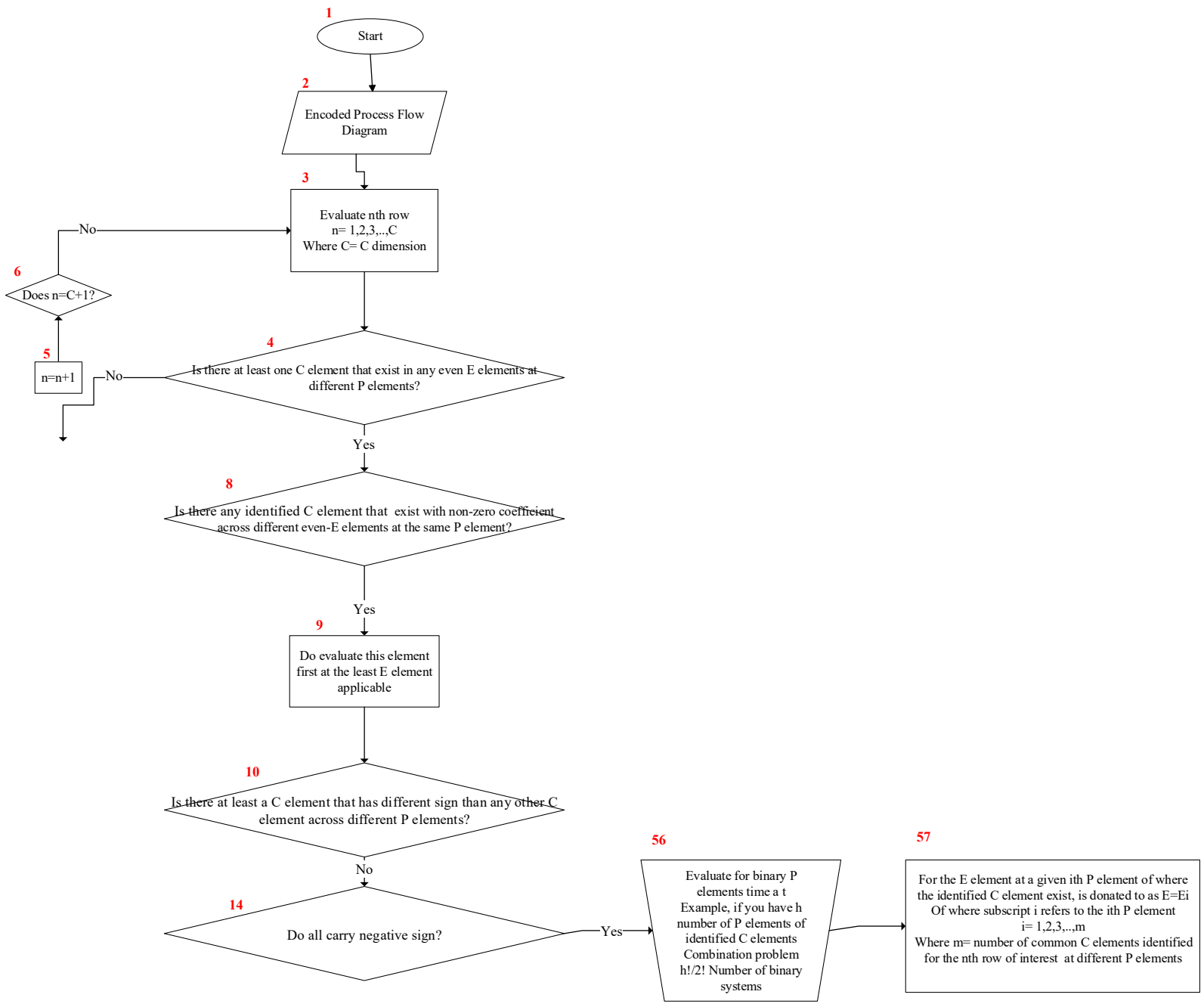

Figure V-9: Flowchart steps applied for part 2, a

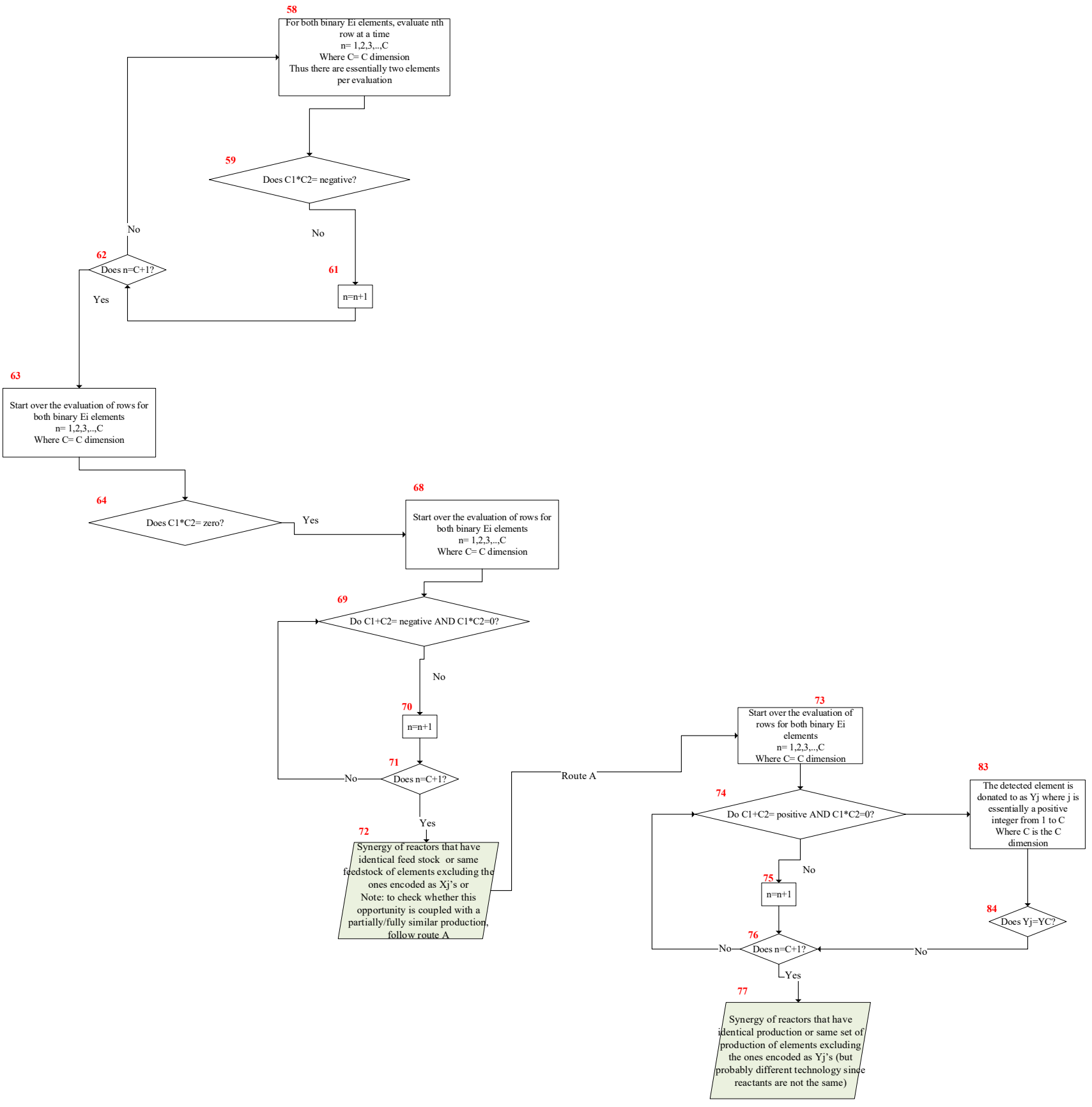

Figure V-10: Flowchart steps applied for part 2, a

The next step is the application of the separation distillation column) algorithm flowchart. The encoded process flow diagram with highlighted steps as per to the separation algorithm flowchart is shown in Figure V-11. Also, the steps of the algorithm that apply to the system are shown in Figure V-12. In the first step of the flowchart, a manual loop asks to evaluate all possible binary combinations of elements. Thus, every combination of columns multiplied by every possible combination of rows of binary combinations is to be evaluated. In this illustration, only two combinations are shown since more combination are found not to bring different results. As shown in Figure V-11, the first two rows combined with the first column of every matrix is evaluated. The highlighted elements in yellow, Acetic Acid and Water are found to be in common, satisfying step 5 with yes. Then, it moves from step 7 to 8 since only one non-unity coefficient exist. Then, at step 7, it eventually identifies that the non-unity coefficient is not being separated into pure component at any stage of the process. Thus, it results of terminating the round to another round via the manual loop until all combinations are evaluated. Ultimately it would terminate the flowchart since no satisfactory combination is available. Thus, it can be stated that no synergy of separation type is available by the current system of interest, namely between Ethanol and Acetic Acid plants considered in this case study.

Encoded Ethanol Plant							
	1 (column)	2 (reactor)	3 (column)	4 (reactor)	5 (column)	6 (reactor)	7 (column)
AcOH	**2**	5	2	-5	0	0	0
H2O	**1**	0	1	6	0	0	21
MeOAc	-2	2	-1	2	1	-1	0
MeOH	-1	-1	12	-2	21	2	-1
CO	0	-2	0	0	0	0	0
H2	0	0	0	0	0	-2	0
MeI	-3	0	0	0	-1	0	0
EtOH	0	0	0	0	0	1	1
LiI	0	0	0	0	0	0	0

Encoded Acetic Acid Plant		
	1 (column)	2 (reactor)
AcOH	**1**	1
H2O	**-1**	0
MeOAc	-3	0
MeOH	-2	-1
CO	0	-2
H2	0	0
MeI	-4	0
EtOH	0	0
LiI	0	0

Encoded Ethanol Plant							
	1 (column)	2 (reactor)	3 (column)	4 (reactor)	5 (column)	6 (reactor)	7 (column)
AcOH	**2**	5	2	-5	0	0	0
H2O	1	0	1	6	0	0	21
MeOAc	**-2**	2	-1	2	1	-1	0
MeOH	-1	-1	12	-2	21	2	-1
CO	0	-2	0	0	0	0	0
H2	0	0	0	0	0	-2	0
MeI	-3	0	0	0	-1	0	0
EtOH	0	0	0	0	0	1	1
LiI	0	0	0	0	0	0	0

Encoded Acetic Acid Plant		
	1 (column)	2 (reactor)
AcOH	**1**	1
H2O	-1	0
MeOAc	**-3**	0
MeOH	-2	-1
CO	0	-2
H2	0	0
MeI	-4	0
EtOH	0	0
LiI	0	0

Figure V-11: Application separation Algorithm Flowchart to the case study SAMPLE

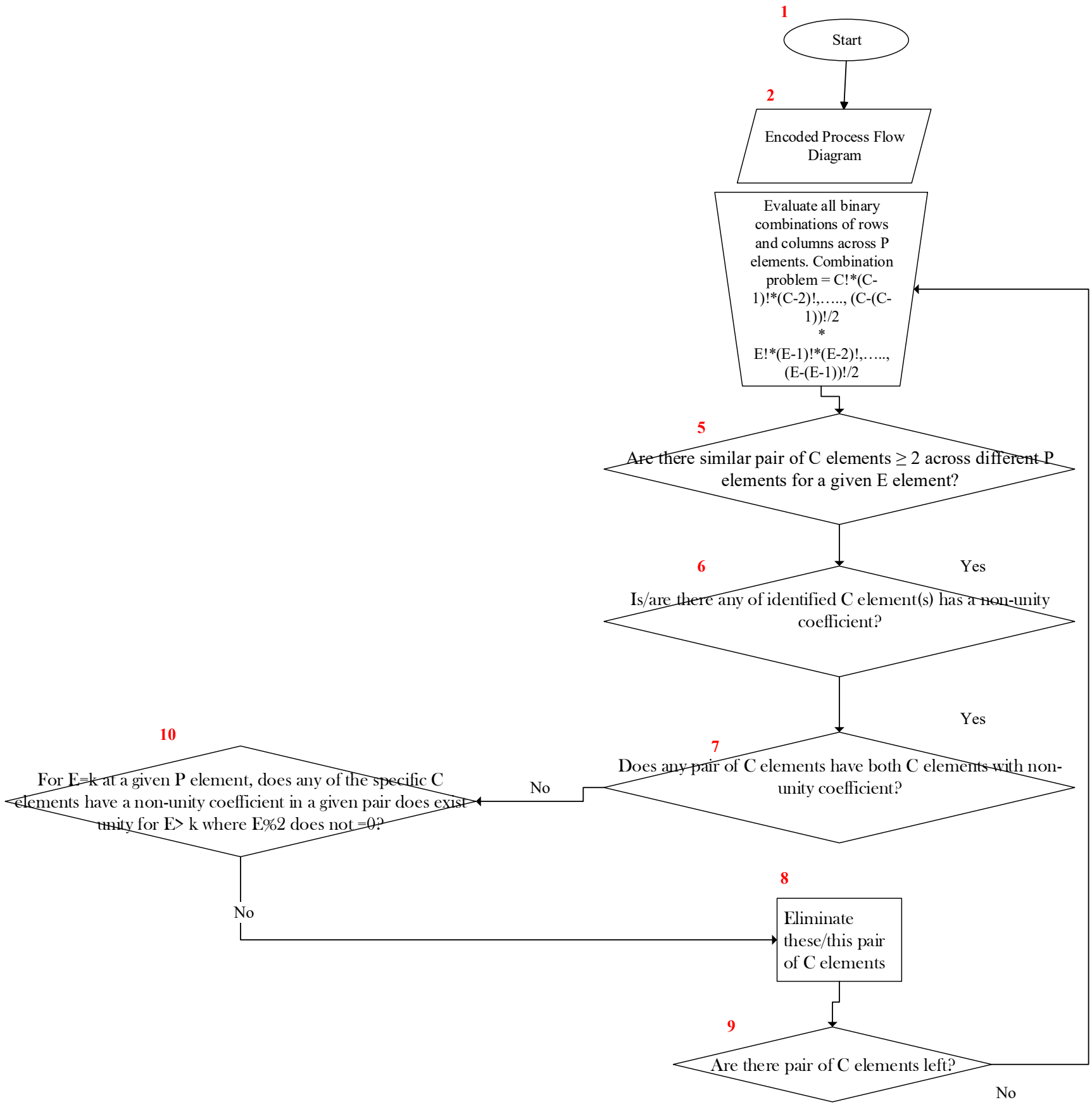

Figure V-12: Flowchart steps applied for separation algorithm flowchart

The standalone plants are subjected to the developed flowcharts. Three synergy type are found by the reactor algorithm flowchart, while no synergetic opportunities are found by the separation flowchart. The following points list the synergetic opportunities that are identified: Note that part of the statement is eliminated, adjusting it to the given case.

- There is Synergetic Opportunity to partially/fully similar system of reactions
- Synergy of reactors that have identical feed stock of elements
- Synergy of reactors that have partially similar set of production

This synergy type is to be utilized in order to come up with a proper design in the plant to integrate based on the identification. The following section shows the reasoning behind the implementation of the synergy opportunity that is identified.

CHAPTER VI

ILLUSTRATIVE EXAMPLE PART III: STRUCTURALLY INTEGRATED PLANT DESIGN PHASE

In this section, the plant design traditional phases are conducted to the structurally integrated plant. First, the plant needs to be designed by defining its structure. This design activity is restricted by product capacity and quality. Additional to the traditional approaches that can be used to design the plant, hereby, new three factors are made available by the developed systematic approach towards integrating processes in terms of their structure. In the previous sections, three synergy types were identified. The first one is a synergy that specifically highlights an opportunity of utilizing commonalties in specific reactor operation that results from utilization of a side product. This specific message is not told by the final statement of the synergy but it is found in the message that is available to the user before the synergy general statement is stated. The second and third synergetic opportunities highlight the fact that there is one reactor that has identical feed which also has partially similar production. In the context of the process, the first synergy considers the utilization of Acetic Acid to further produce Methyl Acetate, of where the latter is a main reactor product and does exist in the original reactor of where the side product, Acetic Acid, is produced. The second and third synergy types highlight the Carbonylation reactors of the two processes. As it is shown earlier, Carbonylation reactors are not identical. Although they similar solvent components, with different compositions, close operating conditions, and identical feed, they have different production. While considering these two factors in designing the structure of the new plant, the following scenarios could be obtained, and hence using the identified synergetic opportunities can be utilized from two perspectives:

1. Elimination of Carbonylation reactor at ethanol plant and supply the missing need of acetic acid by acetic acid plant to produce the needed amount to supply the Hydrogenolysis section with Methyl Acetate
2. Elimination of esterification section and manipulate the production capacity of the two plants to satisfy the individual productions.

Hereby, scenario number 1 is implemented. The first task is to scale up the Acetic Acid Plant which is done as follows:

The scaling up should be done carefully, of where not only the minimum production for the original plant needs to be satisfied but also the capacity of the plants should not be over inflated. This is important on order to account for same degree of purity and recovery for the purification and separation units, recycles, and solvents in the plant. For example, if the capacity is large enough to be sufficient to supply the plants with poor recovery. Here a consistency problem may raise up. Thus, the modified capacity is kept to the most possible minimum to mimic a proper integrated plants with almost same overall capacities.

Scaling-up the capacity of Acetic Acid Plant and Esterification reactor provide the designer with the mass balances needed to design these two reactors, while the hydrogen lysis reactor is kept the same. The following steps summarize the scaling-up procedure:

1. In order to know the new capacity needed for Acetic Acid Plant, the needed amount of Acetic Acid to generate same amount of Methyl Acetate as in the original Carbonylation reactor needs to be determined.

2. Because the Carbonylation reactor of Ethanol plant is eliminated, its main production and the consequence of its production needs to be satisfied.

3. The main product of Carbonylation reactor of Ethanol plant is Methyl Acetate, because Acetic Acid is produced as a side product and it is further processed to produce acetic acid, this synergy is converted into the following scenario:

4. the overall Methyl Acetate that enters the Hydrogenolysis section of Ethanol plant needs to be the same for the integrated plant. This value is obtained from the stream data from Original Ethanol Plant. This amount is in stream S-302, that is the bottom stream of the distillation column of Methyl Iodide recovery is: 338.6282 kmols/hr. The restrictions to presence of other components follow the restricted ranges within the original study.

5. In order to satisfy point 4, the conversion of esterification reaction is taken into account. The generation of Methyl Acetate from Acetic Acid follows 1 to 1 molar ratio with a conversion of Acetic Acid (limiting reactant) of 95%, with no other side reactions (as in the original case of original Ethanol Plant).

6. According to point 5, the amount that should be sent to Ethanol plant from increased production Acetic acid plant within the integrated structure plant is 1.05 * 339 kmol/hr or (339 + (339*0.05)) to account for the loss due to the non-complete conversion of Acetic Acid.

7. Note that the amount mentioned in point 6 is the separated amount of Acetic Acid original production that is 640 kmol/hr which is actually 637 kmol/hr after separation, accounting for 99% moles recovery at the product column of original acetic acid plant.

8. For the integrated plant, if a mole recovery of acetic acid is assumed to be as one of the original Acetic Acid plant, 99%, then 637 kmol/hr (for AcOH plant) + 356 kmol/hr for the integrated Ethanol is the desired amount after separation. Since recovery is 99 mol%, then the original amount needs to be produced by the reactor is approximately 993 kmol/hr Acetic Acid.

7. It is worth mentioning here that the recovery of acetic acid from the post reactor flash separator is by passed because it is almost 100% in the origin reactor al process.

VI.1 PROCESS DESCRIPTION

This plant produced Acetic acid, Ethanol, and co-produce Methanol of same quantity as well as quality as the stand-alone plants presented earlier. The process starts by feeding Carbon monoxide and Methanol, of where the former is fed in excess, to Carbonylation reactor to convert them into Acetic Acid. The produced Acetic Acid supplies the next reactor, that is Esterification reactor with the needed amount of Acetic Acid that is to be converted to Methyl Acetate, while the leftovers of Acetic Acid represent the production capacity of the original Acetic Acid Plant. At the esterification reactor, Acetic Acid with Methanol is being converted to Methyl Acetate and water. The former product is sent to the Hydrogenolysis section, following the same conditions as the original section at Ethanol stand-alone plant. In the later section, Ethanol as a main product and Methanol as a co-product are obtained. It is worth mentioning here that the Methyl Iodide recovery unit is not needed since the Carbonylation reactor at Ethanol plant is omitted.

The process flow diagram of the structurally integrated plant is shown in Figure VI-1.

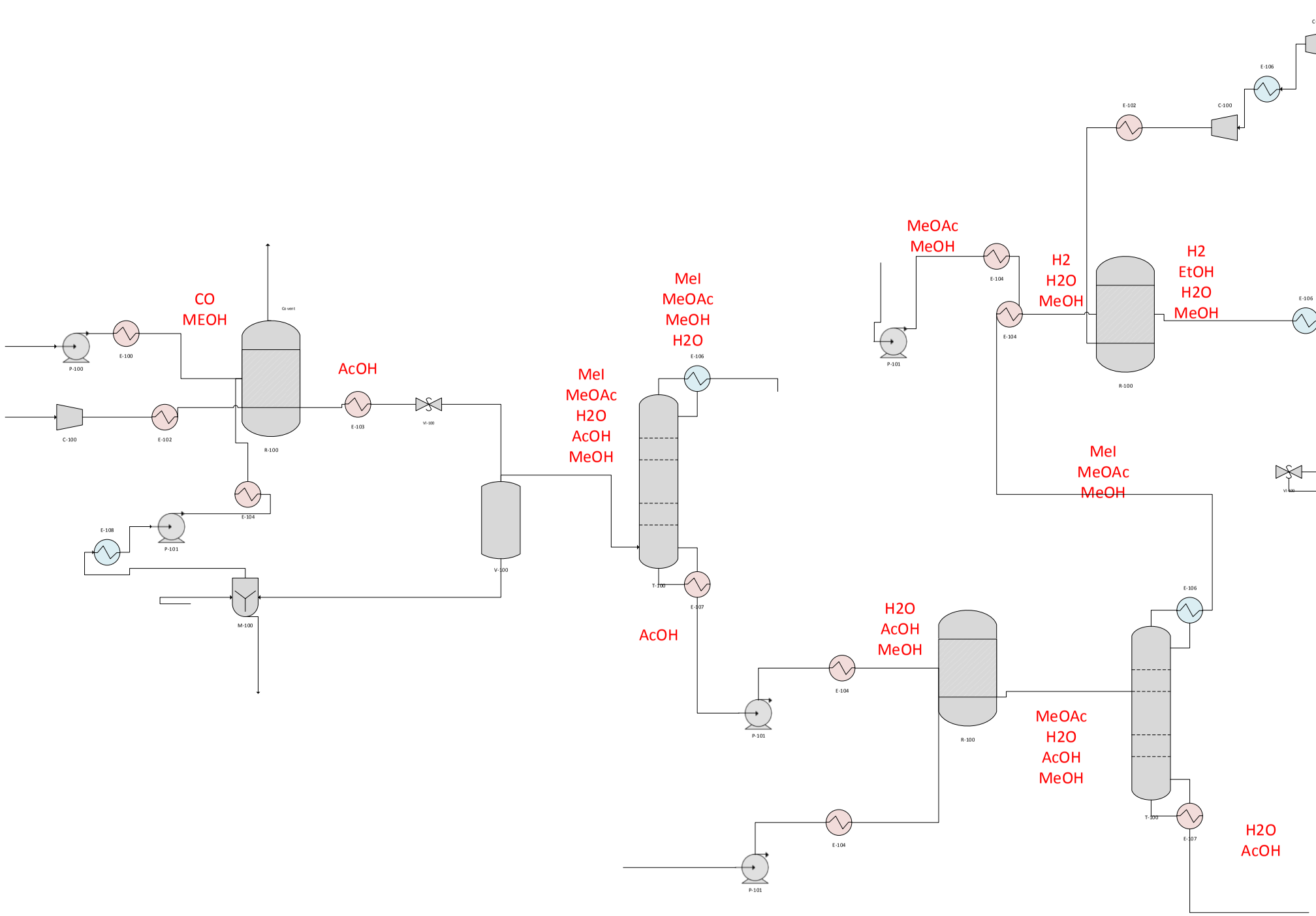

Figure VI-1: Process flow Diagram of Structurally Integrated Plant

VI.2 SIMULATION OF THE STRUCTURALLY INTEGRATED PROCESS

Process simulation is conducted in the same manner as the previously simulated stand-alone units. Steam data and Mass balances can be found in Appendix B.3. Also, the simulated process flowsheet is shown in Figure VI-2. The simulation of the integrated structure starts from the stand alone plants combined in one flowsheet, and the steps of scaling up acetic acid plant are followed. Careful attention is given to the flow of the composition not to exceed the recommended ranges nor deviate from the actual original process. Basically, the process block diagram

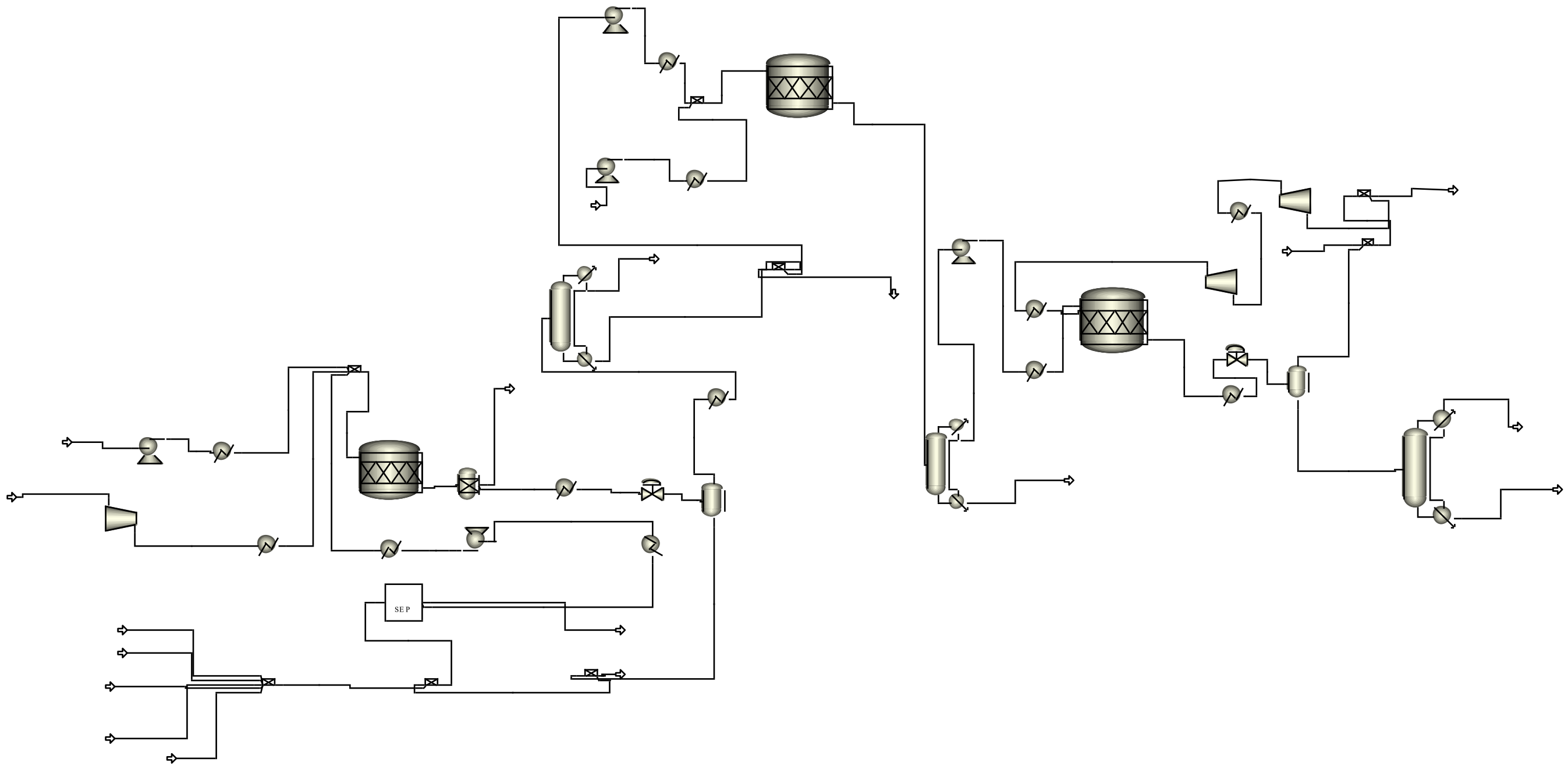

Figure VI-2: Simulation Environment of the structurally integrated plant

VI.3 HEAT INTEGRATION OF THE STRUCTURALLY INTEGRATED PROCESS

Heat Integration for the structurally integrate plant follows the approach that is applied previously to the stand alone plants. The Heat exchanger network design can be found in Appendix F.3 in Tables F-6 and F-7. Utility system is shown in Tables VI-1 and VI-2. Lastly, the performance of heat integration is assessed by the influence of the application of heat integration on cost of various parameters as shown in Table VI-3. The overall Plant simulated flowsheet is shown in Figure VI-3.

Table VI-1: Utility System at Structural Integrated Plant before Heat Integration

	Current	**Target**	**Energy Cost Savings**	**Energy Cost Savings**	**ΔTmin**
	[cal/sec]	**[cal/sec]**	**[$/Yr]**	**[%]**	**[C]**
HP Steam	3.42E+06	4.10E+05	995,645	88.04	10
LP Steam	6.26E+06	3.81E+06	614,903	39.13	10
MP Steam	1.26E+06	1.27E+05	327,933	89.88	10
Total Hot Utilities	1.09E+07	4.35E+06	1,938,480	63.2	
Cooling Water	1.15E+06	1.56E+05	27,758	86.37	5
Air	6.82E+06	8.01E+06	-158	-17.48	10
LP Steam Generation	3.42E+06	0	-854,299	-100	10
MP Steam Generation	1.03E+05	0	-29,923	-100	10
Refrigerant 1	3.61E+06	3.36E+05	1,183,535	90.68	3
Total Cold Utilities	1.51E+07	8.50E+06	326,914	72.02	

Table VI-2: Utility System at Structural Integrated Plant after Heat Integration

	Current	**Target**	**Energy Cost Savings**	**Energy Cost Savings**	**ΔTmin**
	[cal/sec]	**[cal/sec]**	**[$/Yr]**	**[%]**	**[C]**
MP Steam	1.29E+06	0	374,477	100	10
HP Steam	2.24E+06	1.29E+06	310,737	42.09	10
LP Steam	8.43E+05	0	211,629	100	10
Total Hot Utilities	4.37E+06	1.29E+06	896,842	67.72	
U-2	9.24E+06	7.34E+06	-472,612	-20.49	10
Air	3.32E+06	2.44E+06	117	26.58	10
Refrigerant 1	7.56E+05	4.59E+05	107,508	39.29	3
Total Cold Utilities	1.33E+07	1.02E+07	-364,987	-17.96	

Table VI-3: Summary of Structurally Integrated Plant Performance influenced by Heat Integration

Name	Before Heat Integration	After Heat Integration	Percentage	Effect
Total Capital Cost [USD]	30155000	33939900	12.6%	Increase
Fixed Cost* [USD/Year]	5095500	4834700	5.1%	Decrease
Total Utilities Cost [USD/Year]	22430200	19080400	14.9%	Decrease
Equipment Cost [USD]	8262900	8864000	7.3%	Increase
Total Installed Cost [USD]	13604000	15163600	11.5%	Increase

*Fixed cost is calculated as Operating Cost-Utilities cost as defined by Aspen Plus™ V.8.1

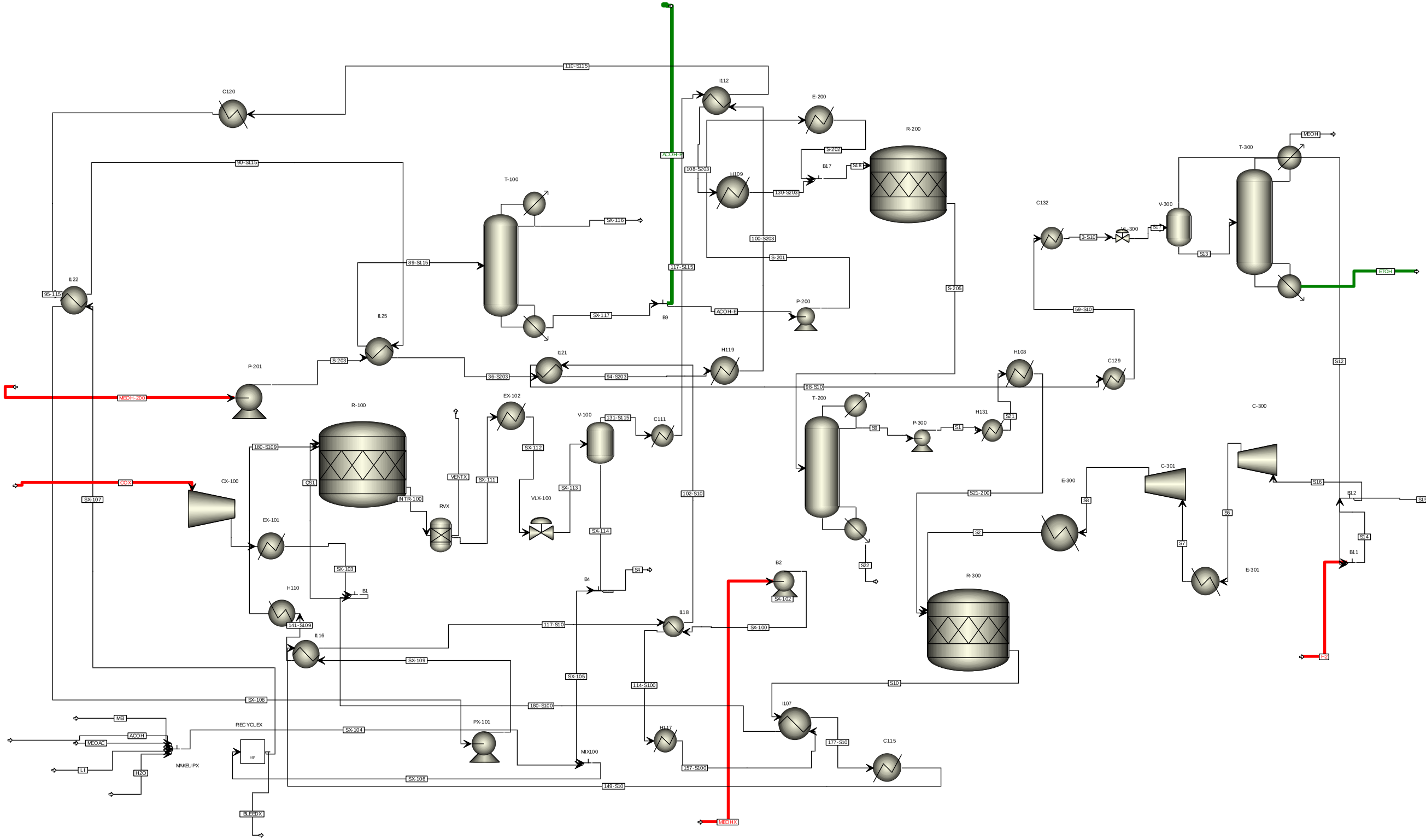

Figure VI-3: Heat Integration simulation view of the structurally Integrated Plant

VI.4 ECONOMIC EVALUATION OF THE STRUCTURALLY INTEGRATED PROCESS

The plant performance in terms of economics can be evaluated by following same procedure as in economic evaluation of the two stand-alone plants. Similar to the stand-alone units, the overall performance of the plant is summarized in the following Table VI-3 after completing the design phase. Also, Table VI-4 shows the Raw material cost at the structural integrated plant.

Table VI-4: overall performance of the plant

	Structurally Integrated Plant
Capital Annualized Cost*	3.40E+06
Utilities Cost	1.91E+07
Fixed Cost**	4.84E+06
Total Annualized Cost	2.73E+07

*Based on Project Life =10 years

**Fixed cost is calculated as Operating Cost-Utilities cost as defined by Aspen Plus™ V.8.1

Table VI-5: Raw material amounts and cost at structural integrated plant

Parameter	Value
Hydrogen approximate, m3/year	64,820,145.60
Carbon Monoxide, Ton/year	284,466.90
Methanol, Ton/year	286,024.11
Hydrogen approximate, $/year	8,750,719.66
Carbon Monoxide, $/year	19,912,683.09
Methanol, $/year	155,184,384.81

CHAPTER VII

INTEGRATED PLANT PERFORMANCE

The analysis of the performance of impact on structurally integrate the two stand-alone plants is evaluated from three perspectives: 1) annualized costs, 2) cost per production capacity, and 3) side effects of the integration. The costs savings are listed in Table 11.1. It should be noted here that the raw material costs are excluded.

As expected form the overall approach of the developed integration type, most savings are directed towards the capital investment with an attractive percent decrease of 31.3%. This saving can be justified by looking deeper into the execution of the identified synergy type. The synergy type identified partially/fully similar reaction systems. This synergy is used as a factor while designing the structurally integrated plant. As addressed earlier in this work, number of scenarios can be generated out of this synergy, however, the scenario that is used is thought to be the one that brings reasonable benefits. Since the specific savings of annualized costs are found to be high for the capital cost, deeper analysis are conducted on the capital cost of the Ethanol plant. Ethanol plant is subjected to this analysis since the eliminated reactor is originally at the Ethanol Plant.

Table VII-1: Annualized Cost Comparison between Structurally Integrated Plants and Stand-alone Plants

	Ethanol Plant	Acetic Acid Plant	Structurally Integrated Plant	Savings
Capital Annualized Cost*	3.45E+06	1.49E+06	3.40E+06	31.3%
Utilities Cost	1.53E+07	5.81E+06	1.91E+07	9.4%
Fixed Cost**	4.85E+06	2.64E+06	4.84E+06	35.4%
Total Annualized Cost	2.36E+07	9.94E+06	2.73E+07	18.5%

*Based on Project Life =10 years

**Fixed cost is calculated as Operating Cost-Utilities cost as defined by Aspen Plus™ V.8.1

First, the reactor itself is analyzed. Savings that are obtained may be justified because a lower conversion reactor is being replaced to a high conversion one (esterification). This also holds for the reaction stoichiometry. The Carbonylation of Methanol to Methyl Acetate consumes two moles of Methanol to produce one mole of Methyl acetate. These aspects give benefit of conducting the Carbonylation at Acetic Acid Plant and the Esterification reactor at Ethanol plant with an adjusted capacity to justify the removal of the Carbonylation reactor at the later plant. Other aspects to analyze the source of savings can be obtained. Figure VII-1 shows the break-down of the direct cost of equipment at Ethanol Plant. A shown, compression as well as distillation account for the highest capital costs in the plant in terms of percentages. It is worth mentioning that compression cost mat be reduced in case the Carbonylation reactor operates at lower pressure, which may be a valid option. The Carbonylation section at Ethanol Plant participates in these percentages of where up to 21% of compression capital cost of the plant result from Carbon dioxide compression at the Carbonylation section. Also, high percentage up to 13% of the capital cost that is associated with the purification units is caused by purification of mostly stream that result from the Carbonylation section, namely column T-100 that produces the first methyl acetate stream and the Methyl Iodide recovery unit. Despite the fact that the removal of the Carbonylation section does not satisfy the needed production

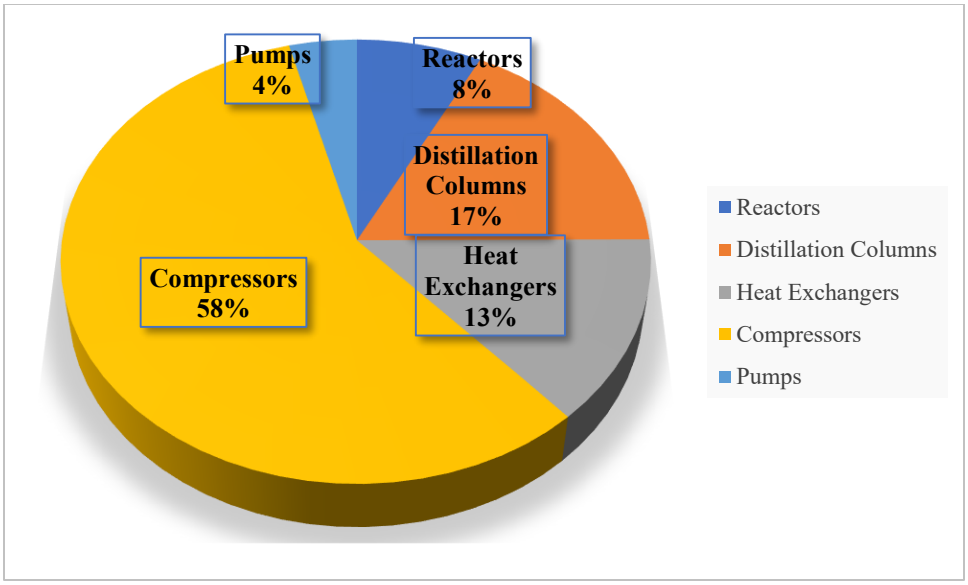

Figure VII-1: Total Equipment Cost Break-down, Ethanol Plant

rate unless it is substituted by an increased production from other reactors in the plant itself and at the other plant, it is believed that its removal would still result in saving due to the following analysis. The compression that is saved by this elimination requires two stage compression, and consequently an intermediate cooler, while one stage compression is needed by the other Carbonylation reactor (at the Acetic Acid plant) which its capacity was adjusted to substitute the needed Acetic Acid by the esterification section after the removal of Carbonylation reactor at Ethanol plant. The number of stages is selected according to the operating pressure, and hence it is worth mentioning here that these pressure values were selected from a range and may be modified to increase or decrease. Yet, the initial selection of these values is done before performing the structure integration, and hence was not influenced by it but this selection has benefited the case. The other aspect is related to the purification units. The first distillation column that recovers Methanol and lighters at the top while recovering acetic acid and water at the bottom is totally

removed. Not only this column, but also, because this column recovers Methyl Acetate along with an amount of Methyl Iodide (comes from the solvent), subsequently, an entire recovery unit of Methyl Iodide is needed. By the elimination of the reactor, the Methyl Iodide recovery unit is eliminated. This does not only add a value to the capital cost but also to other themes. The other themes in this context can be safety and quality. When Methyl Iodide, a toxic chemical, is removed, safety practice is enhanced. Also, Methyl Iodide is a contaminant to the Hydrogenolysis section which make the option of operating with a Methyl Acetate stream that is free from Methyl Iodide stream by default (such as the one at the structurally integrated plant) is beneficial and desired to increase the attention to the quality. This, two more themes are considered in this case study. There are also other themes that are addressed. The reduction in the use of raw material is also accomplished. Hereby, specific raw material savings are calculated to result in 25.3% Carbon monoxide and 7% Methanol. Briefly, the savings that are obtained are analyzed and justified as per to the effect of the removed Carbonylation reactor from the system.

Another calculation that is conducted is the cost per production. Hereby, the cost in $ per Ton of products is conducted as shown in Table VII-2.

Table VII-2: Cost per production capacity comparison

Plant	Total Annualized Cost $/year	Production Capacity, Ton/year		Cost per Production, $/Ton	Reduction
		Ethanol	Acetic Acid		
Acetic Acid	9.94E+06	-	333,685.25	29.79	18.6%
Ethanol	2.36E+07	128,107.20	-	184.22	
Structural Integrated	2.73E+07	127,989.03	333,887.75	59.11	

In Table VII-2, it is expected to have savings as per to the previously analyzed cost savings. This is because the structully integrated plant is contrsained by the production capaicty and quality of main and co-products in the processes. With this resterction, any cost savings will result in an increase in reduction of the cost per production as obtained in the table.

The third aspect that is addressed in the analysis section is related to the side effects that may result from the application of structurally integrated design. A noticed effect in one or more streams in the process, while fixing the constrains of production capacity and quality, is addressed and analyzed in order to provide a precise picture about the integrated process benefits and drawbacks. In ethanol plant, a water stream that is recovered as a result of esterification, contains small amounts of any of unreacted acetic acid. As per to the patent of the technology [22], a water stream results from the esterification may be recovered with high purity, page 16, while in page 5, it is mentioned that any unreacted acetic acid is obtained in the stream of water that was specified with higher limit of 10 wt%. The concentration of acetic acid in water depends on number of factors: the amount of water fed to the reactor since even with increased capacity, the concentrations should stay the same as long as the feed ratio and the conversion are the same. Thus, the reason behind this change in water stream amount is the lack of water fed to the reactor. In the original process, water was not separated from acetic acid before feeding the later into the esterification reactor, and hence, significant amount of water is obtained at the reactor effluent. However, for the case of the integrated structure plant, the acetic acid that is fed to the reactor is almost pure and free of water since it is supplied from the adjusted-capacity acetic acid plant. Thus, the capacity and the quality of this water stream is affected. It is determined by the mass balance of the process. It is worth mentioning that if the conversion that is used for the reactor was higher, the present issue would not exist. Thus, the capacity of water is 6135 kg/hour with concentration

of Acetic Acid of 6 wt% for Ethanol plant, while these numbers are 5810 kg/hour of water with 15.5 wt% Acetic Acid for the structurally integrated plant. Hereby, one additional attempt is made in order to verify the effect of purifying this water stream on the savings, a distillation column is installed and purified the water up to the level stated by the original patent of the technology [22] that is 10 wt%. The simulation results for the water stream are 5511 kg/hour of water with a concentration of 9.3 wt% acetic acid. This simulation influenced the previously stated saving as follows: 27.2% annualized capital cost, 33% fixed cost, 0.5% utility cost, with total annualized cost of 11.7 %. Regardless the effect on the cost, one benefit that can obtained is the purified Acetic Acid stream that can add to the production or raw material. Briefly, this aspect is addressed to provide a comprehensive picture about the effects of the approach application. In general, since no explicit statement was made referring to this water stream for either being a main product, co-product, or a process specification that affect the consequences of the process, the original flowsheet is maintained the same, and the results are obtained accordingly.

The details of the costs mentioned here are available in the Appendix E.

CHAPTER VIII

CONCLUSION

This work is implemented with a focused target in contributing to enhance the chemical process performance by influencing the design decision-making activity that defines the process structure with a new factor. These factors are generated by moving the design activity in single process synthesis to a level of system of process synthesis. These new factors are believed to provide the design engineer with new opportunities towards a more efficient process design. The research started with reviewing the literature in order to sort-out the developed attempt that share the same global goal (enhance process performance) and to more specifically study the recent development in advances in chemical process synthesis. The review in the literature shows that there is a need to systematically approach process synthesis to more efficient process design. Since the approach of this research is to cross the process boundaries in designing the new process structure, the literature of similar manner has been reviewed, concluding that the developed attempt has mainly contributed in opening the process boundaries with the energy/water systems that lay into the outer two layers of process hierarchy without much of attention into the design of the core structure. These outcomes have developed the motivation towards implementing and formulating an approach that systematically crosses the process boundaries and is able to identify possible opportunities, or possible synergy for structural integration. The research them moved into the formulation phase of where the main elements that contribute to the process design of the core structure where organized into sets with respect to system of n plants participating the integration. The sets include set of plants, equipment and components. These sets are then translated, with special instructions to every synergy type, into encoded process flow diagram in a

matrix form. Every two dimensional matrix represents a chemical plant. These matrixes are used as the main input to the algorithms that search the synergy that may be available in the selected systems. In this work, two synergy types are presented, namely, reactors and separator. Each one of them ends up with either finding identical tasks that take place in among the selected processes, tasks that are partially similar, or tasks that are similar with altering the original design parameters. Also, it emphasized that these algorithms do not suggest a design but the main objective of using them is to find opportunities which may be translated later into multiple design scenarios. The work later moved into the phase of implementing a case study that represents actual processes. Basically, two processes were selected, production of acetic acid and production of ethanol. The initial selection is believed, without deep analysis to result in synergies. The implementation of these plants considered simulation by the use of Aspen Plus. The overall whelming approach is to consistently simulate the plants so that they are evaluated at same levels. Then, a heat integrated approach is applied by a generated heat exchanger network by Aspen Energy Analyzer. Economic Evaluation of the stand-alone units is done, Then, multiple scenarios are generated based on synergy types found to address direct and indirect separation tasks and partially similar reactor task. The later synergy helped in figuring out two main scenarios to alter/synergize the reactor systems. One of the scenario is implements of where one reactor task is completely eliminated, and the production of the missed products where obtained by adjusting the capacity of the leftover reactors. The same design phases were applied to the structurally integrated plant. Then, the overall economic evaluation of the performance of the applied approach is considered. This evaluation resulted in two main conclusion of percent savings that are up to 31% saving in capital cost, while 16% saving in total Annualized cost (annualized cost of operating, utility, and capital costs). A side evaluation was done of the saving on raw material. With respect the obtained process, saving

of CO feedstock reach 25% while 7% for Methanol. These results are justified according to the cost contribution of the eliminated units, and also replacing a weak-productivity reactor to a higher –productivity one. This conclusion is believed to satisfactory hits the target of the study. Since the overall study targets the core structure, then it is expected to have the most savings in the capital cost. This work can be further developed by generating new algorithm for new synergy types and/or adding more routs for the existing synergies.

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APPENDIX A

ALGORITHM FLOWCHART SPECIFICATIONS AND EXPLANATION

Table A- 1: Reference Table to the encoded Algorithm flowchart of Separator

	Role	**Statement**	**Practical Implication**
1	Terminator	Start	The start of the flowchart
2	Data (input)	Encoded Process Flow Diagram	Data input (matrix representation of the plants)
3	Manual Loop	Evaluate all binary combinations of rows across P elements. Combination problem = C!*(C-1)!*(C-2)!,….., (C-(C-1))!/2	This manual loop is considered to evaluate all possible binary combination of rows. The total result of the number of binary combination of rows is provided.
4	Process	Add/change P elements	Termination of the steps due to lack of common components.
5	Decision	Are there similar pair of C elements ≥ 2 across different P elements for a given E element?	This step asks about common two C elements (components) among a binary combination of rows at given distillation columns across Plants.
6	Decision	Is/are there any of identified C element(s) has a non-unity coefficient?	This step asks about whether there is a non-key element among the identified common elements in the previous steps.
7	Decision	Does any pair of C elements have both C elements with non-unity coefficient?	This step checks whether any of the identified is a non-key or not.
8	Process	Eliminate these/this pair of C elements	This is an instruction to eliminate the elements detected as yes out of step 9. The reason behind this is that if two elements are in common but both of them are non-key, then separation expectation for them as being untimely key component is unlikely to take place in reality.
9	Decision	Are there pair of C elements left?	This step checks whether there are leftovers after the elimination of step 10
10	Decision	For E=k at a given P element, does any of the C elements have a non-unity	This element checks the final destination of the common binary elements that contain

		coefficient in a given pair does exist as unity for E> k where E%2 does not =0?	one non-key component among odd columns (separators)
11	Decision	For the given E, are there any other C-elements with non-zero coefficient?	This step asks about whether the identified elements in a given distillation column exist as part of a mixture or as binary mixtures (the identified two elements only)
12	Process	The component identified are ultimately separated into pure components. Basically, they do not present in a mixture and hence the following synergy type exist. However, careful attention should be given to the intermediate components that may exist with an intermediate relative volatility with respect to the identified two elements in common which may limit the structural integration	information about the system before stating the synergy identified
13	Data (output)	There are common separation tasks	This is a synergy output as a result of No response to step 7.
14	Process	Evaluate the rows for both binary Ei elements n= 1,2,3,..,C Where C= C dimension i= ith number of plants i=1,2,3…,P Where P dimension	Instruction for the start of evaluation loop
15	Decision	For given E=m, does C exist at E>m as unity at same P element? Conditions: 1) E%2 does not =0 2) No non-zero other than unity coefficients exist at given E>m	This element checks the final destination of the common binary elements that contain one non-key component among odd columns (separators) The stated conditions can be further illustrated in loop manner. Hereby, they are just directly stated to show the intention of the flowchart.
16	Process	n=n+1	Evaluation of next row in a loop

17	Decision	Does n=C+1?	Check over terminating the loop when the maximum limit is reached (above than the dimension of the system)
18	Process	The component(s) exist with the identified common ones do not, in partial/in total, being separated into pure components. Thus careful attention should be considered in dealing with the other components in the column while conducting the following synergy type. In addition, because the common elements do not present in direct relative volatility split in at least one distillation column, careful attention should be given to the intermediate components that may exist with an intermediate relative volatility with respect to the identified two elements in common which may limit the structural integration	information about the system before stating the synergy identified
19	Process	The components that exist with the identified elements are not, in partial or in total, being separated into pure components. Thus careful attention should be considered while conducting the following synergy type.	Information about the system before stating the synergy identified
20	Process	The components that exist with the identified elements are being separated into pure components.	Information about the system before stating the synergy identified
21	Process	The component identified are ultimately separated into pure components. Basically, they do not present in a mixture and hence the following synergy type exist. However, careful attention should be given to the	information about the system before stating the synergy identified

		intermediate components that may exist with an intermediate relative volatility with respect to the identified two elements in common which may limit the structural integration	
22	Data (output)	There is an opportunity for sharing tasks after altering the separation sequence	Synergy output

Table A- 2: Reference Table to the encoded Algorithm flowchart of Reactors

No.	Role	Statement	Practical Implication
1	Terminator	Start	The start of the flowchart
2	Data	Encoded Process Flow Diagram	Data input of the encoded chemical process flow diagram described in the input primary and advanced subsections
3	Process	Evaluate nth row n= 1,2,3,..,C Where C= C dimension	The main objective is to navigate through rows one by one starting with the first and ending with the largest available row while the use of the rest of the flowchart. The flowing definitions clarify the used terms: - The term evaluate is appreciated a "consider" the following for the coming steps of the flowchart - The "row" represent the C dimension which represents the dimension that is determined by the global; set of chemical species of the participating plants. - The terms "nth, and n=1,2,3,..C" represent the number of the row with a set of the real integer positive number which starts with 1 and ends with C. The largest number of this range is essentially C since the number of row is fixed by the number of chemical species in the system, in other words C - dimension
4	Decision	Is there at least one C element that exist in any even E elements at different P elements?	The objective is to find chemical species that exist in 1) reactors and 2) across multiple plants. The following reasoning is considered: - Search is instructed across different P elements (different plants) - Search is conducted over even E elements (E elements: the columns, E dimension, that represent the equipment in general, while even specification to

			direct the search to the reactor equipment type)
5	Process	n=n+1	This is the NO consequence of step 4. The objective is to search through the next row. The row execution is explained in step 3. In this instruction, the nth row moves to the next row by addition of 1.
6	Decision	Does n=C+1?	The objective is to check the satisfactory of range of C rows
7	Process	Add/change P elements	This is the YES consequence of step 6. The objective is to exist the loop when all rows are evaluated back to the start f the flowchart. In specific, the process states the instruction to change and/or add a P element of where the preceding steps did not result in synergy.
8	Decision	Is there any identified C element that exist with non-zero coefficient across different even-E elements at the same P element?	The objective of this step is to consider the case of possibility of identification of an element that exist in multiple reactor within the same plant. Here, the existence is stated as non-zero coefficient within the matrix. This is important to avoid dual consideration of a given element in a given column (reactor)
9	Process	Do evaluate at the least E element applicable	This is the YES consequence of step 8. The objective is to provide an instruction for a special case. The case is the presence of common element (presence=element has a non-zero coefficient) at different "places" within one row. In this context "pleases" refer to columns that are essentially the E elements. If this case is valid, then the C element that exist at the least column should be considered for the following steps in the flowchart.
10	Decision	Is there at least a C element that has different sign than any other	The objective of this is to identify the chemical species that are being consumed and/or produced. Specifically, it asks about the existence of at least one component that exist with two different signs,

		C element across different P elements?	and hence the component identified in common across plants is being produce d in one plant while being consumed in the other. This identification is important for the following steps.
11	Decision	Is the number of all C elements of interest >2?	Because the output of the algorithm flowchart does not provide a synergy that directly comes out of a reactant that presents as a product in another plant and vice versa, the case if only 2 components are detected with opposite signs has a special consideration.
12	Process	Since the number of C elements is essentially 2, then there is one negative and one positive sign-elements. Here is a possibility for synergy of opposite operations. Following the next steps verify over the validity of this option.	This step provides instructions and clarifying situation about the system and the following route. In this step, since the system detected a number of 2 elements with negative signs, then there a possibility for opposite task synergy. Thus, it sends the data to step 56 that is followed by a loop which verifies the stated option.
13	Process	If the system of P elements contains minimum of 2 negative signs, you may exclude all other positive and chose route A, while route B for the opposite. Otherwise, you may chose route C to evaluate with different signs	This block provides the user with clarification about the situation and available options. It simply directs the case into 3 routes. Since there are essentially more than 2 elements with at least one that has a negative sig while there is at least another element that carries a positive sign, then the third one should form a pair of elements that carry same signs. This pair is the minimum condition, and it may be directed to routs A or B for similar signs, or route C for different signs illustrated in step 12
14	Decision	Do all carry negative sign?	This is a subsequent more specific question to YES response to step 10
15	Decision	Do all carry positive sign?	This is a subsequent more specific question to NO response to step 14
16	Decision	Is there at least one C element that has a unity coefficient?	This question results from the YES response of step 15. The objective is to identify the specific

			product type. First priority for this algorithm flowchart is given to main-process products.
17	Decision	Is there at least one C element that has a coefficient of 2?	This question results from the NO response of step 16. The objective is to identify the specific product type. Second priority for this algorithm flowchart is given to main-reactor products.
18	Decision	Is there at least one C element that has a coefficient of 3?	This question results from the NO response of step 16. The objective is to identify the specific product type. Third priority for this algorithm flowchart is given to co-products.
19	Data (output)	Up to the range of this algorithm, there is no synergy out of this nth row	This results from responding with NO in step 18. The algorithm flowchart terminates at this stage since by responding NO to each of having a minimum one component of 1,2, and 3 means that they shall be either waste of side products. None of these cases has an identified synergy in this work.
20	Data (output)	An Error has occurred for input data specification. Check you input and execution	This is an error message that pops up in case of wrong input specification. In this case, an error appears because there only three cases valid in the context of signs that are all components with negative signs, positive signs, or different signs. If none of these is selected then there is an error.
21	Decision	Is the output >1? Where the number of outputs is essentially positive integer	This is the result of YES response to step 16. In this case, there is at least one component of the identified ones acquire a unity coefficient (main process product). Thus, because it asks about the least, there is a possibility to have multiple outputs. The latter case requires special considerations since the unity coefficient is unique to the process main production. If the same component has a unity coefficient across plants, then the plants have same main production which is the case that is addressed later.
22	Process	The processes of the P elements that contain C elements with	The objective of this step is to briefly inform the user about the result of responding YES to step 21

		unity coefficients have same production. The following route verifies over the input of identical processes or same production by different technologies	(explained in detail in step 21 in this table), and directs the flowchart to another area that identifies over the identical plants/processes or processes that have same main production but with different technologies. A different technology is defined as totally/partially different feedstock.
23	Process	The P element that contains the identified C element in the previous step is donated to as the original P element	This step is needed in case the response of step 21 is NO. If the response is NO, then there essentially one element with one unity coefficient. The objective is to encode the plant name that contains such element for later differentiations. In this case it is called the original P element
24	Decision	For C elements belong to P elements other than the original one, does any has a coefficient of 5 to infinity?	The objective if it is to verify the contribution of the other component whether being a side product or not. Because as defined earlier, every side product per plant is unique, it is given a different number of the set 5 to infinity.
25	Decision	Is there at least one C element that has a coefficient of 3?	This step is the result of the NO response to step 78. It verifies whether the identified component in the secondary P element is a co-product. Thus, it asks about the coefficient of 3. The question about the co-product has the latest priority in the respective of the series of steps before terminating the flowchart back to next row evaluation. This is because it is believed that this results in a traditional integration type. Check step 27.
26	Process	Up to the range of this algorithm, there is no synergy out of this nth row	This step is termination step as a result of NO response to step 25. Because if the element of interest does not hold neither 2,3, nor (5 to infinity) coefficient it means it is a waste that its possible structural integration synergy is not identified in the context of this algorithm flowchart.
27	Data (output)	Up to the range of this algorithm, no synergy is identified, however, possibility of mass-integration among the two	This step is the result of YES response to step 25. Because the two detected components are a co-product in one plant, while being either co/main product in the other plant, it is believed that the

		processes is valid due to co-production in the secondary process of a min product in the original process Otherwise, evaluate the next nth row To verify over common production, check route A in step 30	integration that may be resulted is a traditional mass integration. Then, it further directs the user back to evaluate the next row for the respective system. Otherwise, a check on common production synergy is suggested via one route in the flowchart.
28	Process	The P element that contains the identified C element in the previous step is donated to as the secondary P element and the respective E element as E=k Where k is essentially an even number The coefficient is donated to as X and it is essentially a positive integer any number from 5 to infinity	This step results from the YES response of step 24. The objective is to encode the plant name that contains such element for later differentiations. In this case it is called the secondary P element. It further instructs over the encoded names/symbols related E and C elements. It instruct to donate the coefficient of the identified element with symbol X, while the column that contains this element as column k, that is E=k.
29	Decision	Does the C element exist at an E element, where E > k AND E%2==0	This step is the consequent step to step 28. It checks over the existence of the identified component in one reactor in the secondary plant in another reactor. This step is needed in order to verify whether the component, that is typically a side product does exist in later stages in the same plant. Furthermore, it restricts the search over the even E elements.
30	Data (output)	Up to the range of this algorithm, no synergy is identified, however, possibility of integration among the two processes is valid due to side-production in the secondary process of a (min/co-product) in the original process	This step is the result of NO response to step 29. It terminates the route of side-product utilization to other possible synergy routs because it detects from the previous step that the component of interest does not exist at other reactors in the secondary process, which implies to that the component is not being further utilized in the process.

		Otherwise, evaluate the next nth row Route A You may further verify over similar production via route B	
31	Process	The E element that contains the identified C element in the previous step is donated to as E=j	This step is a consequent step to step 29 with a YES response. It simply encodes the later reactor of where the same component is being identified. This makes the search more practical. It encodes it as E=j.
32	Decision	Does identified C element at E=j carries a negative sign?	This step is a consequent step to step 31. It checks over the identified side product in secondary plant whether it is further utilized,0 more specifically, consumed in a chemical reaction. Thus, it asks about the sign of the element in the later reactor (i.e. E=j)
33	Decision	Does identified C element at E=j carries a coefficient of X ? X is defined in the preceding steps	This step is a consequent step of step 32. After the sign is checked of the element at the other reactor (i.e. E=j) it checks over the magnitude. In this case the magnitude is critical. It asks whether the magnitude is X that is the same value as the one exist in the former reactor (i.e. E=k).
34	Decision	Does identified C element at E=j carry a positive sign?	This step provides a secondary check about the identified element in a higher column (in another reactor). This step checks over the sign of the element to clearly conclude that it is being produced by asking about the positive sign condition.
35	Data (output)	An Error has occurred for input data specification. Check you input and execution ERROR: as long as a non-zero coefficient element exist, it must carry either a negative or positive sign	This is an error message to the user, indicating that the previously made decision/answer is impossible since once the component is classified as “exist” then it can either exist with a negative or a positive sign.
36	Process	Rename j as k where the previous k column is overwritten as j=k	This step is implemented to further check at higher columns (reactors after the previously checked reactor after the former/original reactor)

			in order to make sure whether it is being utilized or not by checking all reaction systems in the given process. Thus, it will use the previously defined E element, k, to represent the new one, that is j, and let the flowchart to identify new j's.
37	Decision	Does j=E+1? Where E represent the E dimension	This step is implemented in order to assure the checking procedure of all E elements (check over all reactors present in a given process). Also, it assures the aspect of exceeding the limit of the E dimension to decide on terminating the loop or process to a further check.
38	Data (output)	Up to the range of this algorithm, there is no synergy out of this nth row	This step provides a message to the user about terminating the previous loop due to lack of opportunities for the verified system. This is because if the component is not being detected as consumed (carries negative sign in a given column at a given plant), the utilization-based synergy type will not be valid.
39	Data (output)	In case the side product identified and produced in the process is not further consumed in a chemical reaction, but rather, probably, a fresh feed of it is used, up to the range of this algorithm, no synergy is identified, evaluate the next nth row	This step, output, is implemented to inform the user that the flowchart has detected that the element of interest, that is to be checked over being utilized in the plant or not, does present. However, it presents as a fresh feed, according to the specification of the user. This is because the coefficient X is instructed to be kept for the reactant that comes from the process itself. IN this case, since the coefficient s not X, then it is concluded to be otherwise, without further check, by default either 1 or 2. A further check steps maybe conducted and an error message can be written to the user in case none of the 1 nor 2 acquires a positive response form the user.
40	Decision	Does any of the positive C element at E=j has a unity coefficient?	In this step, that is the result of the YES response to step 33, it checks about in what the component of interest is being utilized. In other words, it

			checks whether it is further utilized to produce a main coproduct, co-product etc. Hereby, it checks over the production of a main-process product.
41	Decision	Does any of the positive C element at E=j has a coefficient of 2?	In this step, after assuring that the original identified common element is being further utilized in the process, the system checks over the production of the reactor of where the former element is being consumed in. This step comes after the NO response of step 40, and it has a second priority relative to it. Hereby, the check is made over the coefficient of 2, that is the coefficient for a main-reactor product.
42	Decision	Does any of the positive C element at E=j has a coefficient of 3?	This step works on the same principle explained earlier in steps 40 and 41. The only difference that it has a third priority over them since it asks about the co-production (carries a coefficient of 3).
43	Decision	Does it present at E=k?	This step is the result of the YES response to step 40. It asks about whether the produced main-process product (identified in the step 40) that is being produced by the utilization of the side product (od coefficient X identified earlier) does actually exist in the former reactor in the same plant or not. Thus, it asks about the whether it exist in E=k or not.
44	Data (output)	There is a synergy of reactors of opposite operation task	This is a synergy output block stating the synergy that is identified. Hereby, the synergy identified is related to the type of dual opposite task elimination, with specific type of opposite reactor operations. Specific description about the system is provided in the previous step of a process block of number 87.
45	Process	Applying the following identified synergy should carefully consider the other species being produced at E=k	Message to the user before stating the identified synergy type. Results from step 45.

46	Decision	Does it present at E=k?	This step is the result of the YES response to step 41. It asks about whether the produced main-reactor product (identified in the step 41) that is being produced by the utilization of the side product (od coefficient X identified earlier) does actually exist in the former reactor in the same plant or not. Thus, it asks about the whether it exist in E=k or not.
47	Decision	Does it exist with positive coefficient at E=k?	This step is a consequent step to step 46. It checks whether it was originally produced in the former reactor.
48	Data (output)	The case seems to be un-clear since a component is being consumed in a former reactor in the process and then consumed in another reactor to produce a main product with respect to the later reactor. Up to the range of this algorithm, such case is not covered to yield a synergetic opportunity, evaluate the next nth row	This is a message to the user about the system, and manually directs the user to the start of the flowchart to evaluate next row because the system could not be verified by the limits of the algorithm flowchart.
49	Decision	Does it exist with a coefficient of 2 at E=k?	This step is a consequent step to step 47. It checks over the attribution/role of the component detected in step 47 in the former reactor of the same plant. This is important to see how much significant the later utilization of the side product is.
50	Process	Applying the following identified synergy should	Message to the user before stating the identified synergy type. Results from step 49.

		carefully consider the contribution of the latest C element and other produced species at E=k	
51	Process	This C element is a main product at original P element and a side product at Secondary P element that is being further processed in a chemical reaction to produce the reactor-main product of plant that is represented by secondary P element	Message to the user before stating the identified synergy type. Results from step 49.
52	Decision	Are there any other positive C elements at E=j?	This step results from the YES response of step 43. It checks whether there are any other components present at the other reactor (i.e. E=j). This aspect is being addressed in order to decide of the effect of modifying on this reactor. For example, if other important products exist, integration may be limited.
53	Process	This C element is a main (process/reactor) product at original P element and a product at Secondary P element that is being further processed in a chemical reaction to produce main (reactor/process) product or co-product of plant that is represented by secondary P element	Message to the user before stating the identified synergy type
54	Process	Note: there are other components being produced in the reactor donated E=k and h which may require special consideration while structural integrating the plants	Message to the user before stating the identified synergy type

55	Data (output)	There is Synergetic Opportunity partially/fully similar operations/reactions	This synergy type that is previously explained is obtained via multiple routs in the algorithm flowchart. It results from identification of similar operation in total or in atrial that may lead to partial or total removal/substitution of reactors.
56	Manual Loop	Evaluate all possible combinations of binary P elements Example, if you have h number of P elements of identified C elements Combination problem h!/2! Number of binary systems	This step is implemented in a manual loop block (which may be further developed in an implemented loop). The objective of the step is to instruct the user to evaluate a pair of p elements at a time. For better understanding of the manual execution of this step, the combination problem is stated. This represents the all number of different combinations of binary systems of p elements.
57	Process	For the E element at a given ith P element of where the identified C element exist, is donated to as E=Ei Of where subscript i refers to the ith P element i= 1,2,3,..,m Where m= number of common C elements identified for the nth row of interest at different P elements	In this step, some terms are defined such as the donation to E elements and P elements with eth respective ranges in order to conduct the following steps on clear bases.
58	Process	For both binary Ei elements, evaluate nth row at a time n= 1,2,3,..,C Where C= C dimension Thus there are essentially two elements per evaluation	In this step, an instruction to evaluate pair of E elements at a time (that is two reactors at a time) while scanning over the rows available in the two P elements (two Plants of where the reactors exist)

59	Decision	Does C1*C2= negative?	This step checks over the different in sign across the two element being evaluated at a time. Hereby, when their multiplication gives negative, it means that they have opposite sign. There is no other way for different interpretation in this context.
60	Data (output)	Up to the range of this algorithm, there is no synergy out of this nth row	Message to the user for terminating the flowchart loop of interest.
61	Process	n=n+1	This step provides an instruction to move to the next row of where n is defined in the preceding process block within the respective loop as the number of rows with range from 1 to C where C is the C dimension.
62	Decision	Does n=C+1?	This step checks over the maximum limit of row available in the system. C is already defined as the C dimension, that is the number of components exist in the system that accordingly define the number of rows since rows are pre-defined to represent the C dimension. Hereby, where C column (last row in the given matrix) is reached, the C+1 does not exist to be evaluated, terminating the loop, or making the decision required for the given case.
63	Process	Start over the evaluation of rows for both binary Ei elements n= 1,2,3,..,C Where C= C dimension	The description provided by process step number 58 is applied here but for starting over the scan over the entire range of n.
64	Decision	Does C1*C2= zero?	This step checks over the existence/absence of one element in one rector relative to the other that is being evaluated in the given binary system of columns (reactors). In this case, if a multiplication of two components in a given row gives zero,

			then either one element exist in one reactor and does not exist in the other or both do not exist assuming that 0*0 =0.
65	Process	n=n+1	Description is provided by step 61
66	Decision	Does n=C+1?	Description is provided by step 62
68	Process	Start over the evaluation of rows for both binary Ei elements n= 1,2,3,..,C Where C= C dimension	The description provided by process step number 58 is applied here but for starting over the scan over the entire range of n.
69	Decision	Do C1+C2= negative AND C1*C2=0?	This step checks in a more specific/advanced step relative to step 64. Hereby, the check is made to identify the source of the zero output obtained by some rows from the loop of the step 64. Here, this step subjects the negative components (reactants) to perform the check. Thus, the calculation required is divided into two equations: if the addition of two elements (that essentially have same sign, since opposite sign elements do not reach this step) is negative while their multiplication is zero, then there is for sure one element is zero while the other has a negative sign.
70	Process	n=n+1	Description is provided by step 61
71	Decision	Does n=C+1?	Description is provided by step 62
72	Data (output)	Synergy of reactors that have identical feed stock or same feedstock of elements excluding the ones encoded as Xj's or Note: to check whether this opportunity is coupled with a partially/fully similar production, follow route A	Synergy output message to user
73	Process	Start over the evaluation of rows for both binary Ei elements n= 1,2,3,..,C Where C= C dimension	The description provided by process step number 58 is applied here but for starting over the scan over the entire range of n.

74	Decision	Do C1+C2= positive AND C1*C2=0?	The description of step 69 applies but with considering positive signs instead of negative signs.
75	Process	n=n+1	Description is provided by step 61
76	Decision	Does n=C+1?	Description is provided by step 62
77	Data (output)	Synergy of reactors that have identical production or same set of production of elements excluding the ones encoded as Yj's	Synergy output message to user
78	Decision	Is there at least one C element that has a coefficient of 2?	This step is the result of the NO response to step 24. It verifies whether the identified component in the secondary P element is a main-reactor product. Thus, it asks about the coefficient of 2. The question about the this product has the second priority in the respective of the series
79	Data (output)	Synergy is identified, a main-reactor product is produced in secondary process of a min/co product in the original process Evaluate the next nth row To verify over common production, check route A in step 30	This step is the result of YES response to step 78. It shows that a common species is detected across two plants being a main reactor product in the first and (main/co) product in the other.
80	Process	This C element is a main (process/reactor) product at original P element and a product at Secondary P element Note: synergy identified is without respect to other chemical species that may be produced	Description about the system prior to the synergy statement for more specific insights an=bout the opportunity.
81	Process	The detected element is donated to as Xj where j is essentially a positive integer from 1 to C Where C is the C dimension	This is the result of the output YES to the question stated in step 69. This step is important to sort out elements that are classified under the category of the response to the respective question for further consideration of the actions/decision for the flowchart.

82	Decision	Does Xj=XC?	This steps implemented in order to check the maximum limit of possible X elements obtained via the respective route. This check is important in order to take the decision/actions following this step accordingly. In case if this question results in a positive response it means that all X elements are involved within the respective consideration in the respective loop.
83	Process	The detected element is donated to as Yj where j is essentially a positive integer from 1 to C Where C is the C dimension	This is the result of the output YES to the question stated in step 74. This step is important to sort out elements that are classified under the category of the response to the respective question for further consideration of the actions/decision for the flowchart.
84	Decision	Does Yj=YC?	The description of step 82 applies with alternating the symbol being used with the one that is used in this step to obtain a precipice statement.
85	Process	The detected element is donated to as Kj where j is essentially a positive integer from 1 to C Where C is the C dimension	This is the result of the output YES to the question stated in step 59. This step is important to sort out elements that are classified under the category of the response to the respective question for further consideration of the actions/decision for the flowchart.
86	Decision	Does Kj=KC?	The description of step 82 applies with alternating the symbol being used with the one that is used in this step to obtain a precipice statement
87	Process	In the evaluated pair of reactors, every element consumed in the first is being produced in the second and vice versa. This leads to an identified synergy that is stated in the following block. However, special attention should be considered while integration to evaluate the attribution of the chemical	Description about the system prior to the synergy statement for more specific insights an=bout the opportunity.

		species as this aspect is not covered for identification here.	

APPENDIX B

MASS BALANCES AND SIMULATION CALCULATIONS DATA

APPENDIX B.1 ACETIC ACID STANDALONE PLANT

Table B- 1: Reaction Solution Composition of Acetic Acid Standalone Plant Calculations

Component	Original Composition by Ref.	Modified Composition according to assumptions	Normalized Composition
Methyl Acetate	0.029	0.029	0.0302
Water	0.02	0.02	0.0208
Methyl Iodide	0.152	0.152	0.1581
Acetic Acid	0.633	0.633	0.6583
Lithium	0.0076	0	0
Iodide	0.12	0	0
Rhodium	0.00055	0	0
Iron (ppm)	0.00029	0	0
Chromium (ppm)	0.00007	0	0
Lithium Iodide	0	0.1276	0.1327
Total	0.96251	0.9616	1

Table B- 2: Pilot Scale Mass balance of Carbonylation Reactor at Acetic Acid Plant Part 1

Component	Feed Ref. [20]				Reaction Solution (Reactor effluent)				Net Reaction Effluent/Production			
	wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	0	0	0	0	0.6583	3.9070	0.0651	0.7494	1	2.33	0.0388	1
Water	0	0	0	0	0.0208	0.1234	0.0069	0.0789	0	0	0	0
Carbon monoxide	0.5034	1.26	0.0450	0.5369	0	0	0	0	0	0	0	0
Methanol	0.4966	1.2432	0.0388	0.4631	0	0	0	0	0	0	0	0
Methyl Acetate	0	0	0	0	0.0302	0.1790	0.0024	0.0278	0	0	0	0
Dimethyl Ether	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Iodide	0	0	0	0	0.1581	0.9382	0.0066	0.0761	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Propionic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lithium Iodide	0	0	0	0	0.1327	0.7876	0.0059	0.0678	0	0	0	0
TOTAL ,if any	1	2.5032	0.0838	1	1	5.9352	0.0868	1	1	2.33	0.0388	1

Table B- 3: Pilot Scale Mass balance of Carbonylation Reactor at Acetic Acid Plant Part 2

Component	$\mathcal{M}$	Liquid Catalyst Solvent Ideal Feed				CO VENT (100%)			
		wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	60.05	0.4374	1.5770	0.0263	0.5469	0	0	0	0
Water	18.02	0.0342	0.1234	0.0069	0.1427	0	0	0	0
Carbon monoxide	28.01	0	0	0	0	1	0.1732	0.0062	1
Methanol	32.04	0	0	0	0	0	0	0	0
Methyl Acetate	74.08	0.0496	0.1789952	0.0024	0.0503	0	0	0	0
Dimethyl Ether	46.07	0	0	0	0	0	0	0	0
Methyl Iodide	141.94	0.2602	0.9382	0.0066	0.1376	0	0	0	0
Hydrogen	2.01	0	0	0	0	0	0	0	0
Ethanol	78.37	0	0	0	0	0	0	0	0
Propionic acid	74.08	0	0	0	0	0	0	0	0
Lithium Iodide	133.85	0.2185	0.7876	0.0059	0.1225	0	0	0	0
TOTAL, if any		1	3.6052	0.0480	1	1	0.1732	0.0062	1

Table B- 4: Scaled-up Mass balance of Carbonylation Reactor at Acetic Acid Plant Part 1

Component	Feed				Reaction Solution (Reactor effluent)				Net Reaction Effluent/Production			
	wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	0	0	0	0	0.6583	83341.98	1387.88	0.7494	1	38432	640	1
Water	0	0	0	0	0.0208	2633.24	146.13	0.0789	0	0	0	0
Carbon monoxide	0.5034	20782.97	741.98	8855.82	0	0	0	0	0	0	0	0
Methanol	0.4966	20505.6	640	7638.60	0	0	0	0	0	0	0	0
Methyl Acetate	0	0	0	0	0.0302	3818.20	51.54	0.0278	0	0	0	0
Dimethyl Ether	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Iodide	0	0	0	0	0.1581	20012.61	140.99	0.0761	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Propionic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lithium Iodide	0	0	0	0	0.1327	16800.06	125.51	0.0678	0	0	0	0
TOTAL, if any	1	41288.5700	1381.9839	16494.4206	1	126606.08	1852.05	1	1	38432	640	1

Table B- 5: Scaled-up Mass balance of Carbonylation Reactor at Acetic Acid Plant Part 2

Component	$\mathcal{M}$	Liquid Catalyst Solvent Ideal Feed				CO VENT (100%)			
		wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	60.05	0.5093	44909.98	747.88	0.6170	0	0	0	0
Water	18.02	0.0299	2633.24	146.13	0.1206	0	0	0	0
Carbon monoxide	28.01	0	0	0	0	1	20782.97	741.98	1
Methanol	32.04	0	0	0	0	0	0	0	0
Methyl Acetate	74.08	0.0433	3818.20	51.54	0.0425	0	0	0	0
Dimethyl Ether	46.07	0	0	0	0	0	0	0	0
Methyl Iodide	141.94	0.2270	20012.61	140.99	0.1163	0	0	0	0
Hydrogen	2.01	0	0	0	0	0	0	0	0
Ethanol	78.37	0	0	0	0	0	0	0	0
Propionic acid	74.08	0	0	0	0	0	0	0	0
Lithium Iodide	133.85	0.1905	16800.06	125.51	0.1036	0	0	0	0
TOTAL, if any		1	88174.08	1212.05	1	1	20782.97	741.98	1

Table B- 6: Selected/best Runs out of Sensitivity Analysis that is conducted for flash separation unit reverse calculation method for Ethanol Plant Carbonylation Section

Thermodynamic Package	Selected Run Number	Temperature, C	Pressure, bar	MeI wt%	AcOH wt%	MeOAc wt%	H2O wt%	MeOH wt%
WILS-HOC	1198	180	1.5	0.2022	0.2085	0.4442	0.1050	0.0402
WILS-HOC	1084	170	1.5	0.2118	0.1876	0.4607	0.1000	0.0400
WILS-HOC	1085	170	1.75	0.2112	0.1839	0.4642	0.1006	0.0401
WILS-HOC	1086	170	2	0.2102	0.1808	0.4675	0.1012	0.0403
WILS-HOC	1087	170	2.25	0.2088	0.1781	0.4708	0.1019	0.0405
WILS-HOC	1088	170	2.5	0.2070	0.1758	0.4739	0.1026	0.0407
WILS-HOC	1089	170	2.75	0.2051	0.1737	0.4770	0.1033	0.0410
WILS-HOC	1090	170	3	0.2029	0.1719	0.4800	0.1040	0.0412
WILS-HOC	1091	170	3.25	0.2005	0.1702	0.4830	0.1048	0.0415
NRTL-HOC*	1198*	180*	1.5*	0.2043	0.2106	0.4362	0.1070	0.0419

*Selected Operating conditions that are best in matching the mass fraction of original reference by reverse calculation method

Table B- 7: generated streams out of flash selected operating conditions at 180 C and 1.5 bar from Table B-6

Stream	134	136	138
wt%			
ACETI-01	0.4282828	0.2106268	0.561853
WATER	0.1121212	0.1069536	0.115292
CO2	0	0	0
CO	0	0	0
METHA-01	0.030303	0.041918	0.023175
ACETATE	0.2515152	0.4361956	0.138182
DIMET-01	0	0	0
IODIDE	0.1070707	0.204306	0.0474
HYDRO-01	0	0	0
ETHAN-01	0	0	0
PROPI-01	0	0	0
LITHI-01	0.070707	2.7521E-21	0.114098
Total Flow kmol/hr	1897.902	687.5756	1210.326
Total Flow kg/hr	100000	38029.58	61970.42
Total Flow l/min	1483.363	219340	983.575
Temperature C	25	102.4328	102.4328
Pressure bar	40	1.498987	1.498987

APPENDIX B.2 ETHANOL STANDALONE PLANT

Table B- 8: Mass Balance of Carbonylation Section at Ethanol Standalone Plant Part 1

Component	$\mathcal{M}$	Feed				Reactor Effluent (stream 134)			
		wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	60.05	0	0	0	0	0.4283	42828.28	713.21	0.3758
Water	18.02	0	0	0	0	0.1121	11212.12	622.20	0.3279
Carbon Dioxide	44.01	0	0	0	0	0	0	0	0
Carbon Monoxide	28.01	0.5120	22715.58	810.98	0.5455	0	0	0	0
Methanol	32.04	0.4880	21653.19	675.82	0.4545	0.0303	3030.3	94.58	0.0498
Methyl Acetate	74.08	0	0	0	0	0.2515	25151.52	339.52	0.1789
Dimethyl Ether	46.07	0	0	0	0	0	0	0	0
Methyl Iodide	141.94	0	0	0	0	0.1071	10707.07	75.43	0.0397
Hydrogen	2.01	0	0	0	0	0	0	0	0
Ethanol	78.37	0	0	0	0	0	0	0	0
Propionic acid	74.08	0	0	0	0	0	0	0	0
Lithium Iodide	133.85	0	0	0	0	0.0707	7070.7	52.83	0.0278
TOTAL, if any		1	44368.77285	1486.80	1	0.9999999	100000	1897.77	1

Table B- 9: Mass Balance of Carbonylation Section at Ethanol Standalone Plant Part 2

Component	$\mathcal{M}$	Product (Stream 136)				Liquid Catalyst/solvent recycle (Stream 138)			
		wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	60.05	0.2106	8010.05	133.3896543	0.1940	0.5619	34818.2354	579.82	0.4791
Water	18.02	0.1070	4067.400487	225.7158983	0.3283	0.1153	7144.72	396.49	0.3276
Carbon Dioxide	44.01	0	0	0	0	0	0	0	0
Carbon Monoxide	28.01	0	0	0	0	0	0	0	0
Methanol	32.04	0.0419	1594.12	49.75418023	0.0724	0.0232	1436.18	44.82	0.0370
Methyl Acetate	74.08	0.4362	16588.33547	223.9246148	0.3257	0.1382	8563.18	115.59	0.0955
Dimethyl Ether	46.07	0	0	0	0	0	0	0	0
Methyl Iodide	141.94	0.2043	7769.67	54.73912478	0.0796	0.0474	2937.40	20.69	0.0171
Hydrogen	2.01	0	0	0	0	0	0	0	0
Ethanol	78.37	0	0	0	0	0	0	0	0
Propionic acid	74.08	0	0	0	0	0	0	0	0
Lithium Iodide	133.85	2.7521E-21	1.04661E-16	7.81929E-19	1.13731E-21	0.1141	7070.71	52.83	0.0436
TOTAL, if any		1	38029.58	687.5234724	1	1	61970.42	1210.25	1

Table B- 10: Mass Balance of Esterification Reactor at Ethanol Standalone Plant

Component	Feed				Methanol Feed				Product			
	wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	0.6616	8032.34	133.76	0.3724	0	0	0	0	0.0158	401.62	6.69	0.0086
Water	0.3299	4005.74	222.29	0.6189	0	0	0	0	0.2473	6295.59	349.37	0.4508
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	0.0082	99.98	3.12	0.0087	1	13322.23	415.8	1	0.3673	9350.80	291.85	0.3766
Methyl Acetate	5.46E-06	0.0663	0.0009	2.49E-06	0	0	0	0	0.3697	9413.62	127.07	0.1640
Dimethyl Ether	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Iodide	0.00027	3.38	0.0238	6.63E-05	0	0	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Propionic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lithium Iodide	0	0	0		0	0	0	0	0	0	0	0
TOTAL, if any	1	12141.50	359.2	1	1	13322.23	415.8	1	1	25461.62	774.98	1

Table B- 11: Mass Balance of Hydrogenolysis Reactor at Ethanol Standalone Plant

Component	Feed 1 (Methyl Acetate)				Feed 2 (Hydrogen)				Product			
	wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	0	0	0	0	0	0	0	0	0	0	0	0
Water	0.0101	273.32	15.17	0.0373	0	0	0	0	0.0061	273.32	15.1677	0.0040
Carbon Dioxide	0	0	0	0	0	0	0	0	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	0.0622	1681.68	52.49	0.1292	0	0	0	0	0.2671	11991.95	374.28	0.0987
Methyl Acetate	0.9277	25093.12	338.73	0.8335	0	0	0	0	0.0279	1254.66	16.94	0.0045
Dimethyl Ether	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Iodide	4.46E-05	1.21	0.0084	2.09E-05	0	0	0	0	2.68E-05	1.21	0.0085	2.24E-06
Hydrogen	0	0	0	0	1	6808.47	3387.3	1	0.1372	6161.67	3065.51	0.8081
Ethanol	0	0	0	0	0	0	0	0	0.5616	25218.96	321.79	0.0850
Propionic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lithium Iodide	0	0	0	0	0	0	0	0	0	0	0	0
TOTAL, if any	1	27049.33	406.39	1	1	6808.47	3387.3	1	1	44901.76	3793.69	1

APPENDIX B.3 STRUCTURALLY INTEGRATED PLANT

Table B- 12: Adjusted Production Capacity of Acetic Acid for the Structurally Integrated Plant Part 1

Component	$\mathcal{M}$	Feed				Reaction Solution (Reactor effluent)			
		wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	60.05	0	0	0	0	0.6583	102909.40	1713.73	0.7494
Water	18.02	0	0	0	0	0.0208	3251.48	180.44	0.0789
Carbon Monoxide	28.01	0.5034	33187.81	1184.86	0.5369	0	0	0	0
Methanol	32.04	0.4966	32744.88	1022.00	0.4631	0	0	0	0
Methyl Acetate	74.08	0	0	0	0	0.0302	4714.65	63.64	0.0278
Dimethyl Ether	46.07	0	0	0	0	0	0	0	0
Methyl Iodide	141.94	0	0	0	0	0.1581	24711.26	174.10	0.0761
Hydrogen	2.01	0	0	0	0	0	0	0	0
Ethanol	78.37	0	0	0	0	0	0	0	0
Propionic acid	74.08	0	0	0	0	0	0	0	0
Lithium Iodide	133.85	0	0	0	0	0.1327	20744.45	154.98	0.0678
TOTAL, if any		1	65932.69	2206.86	1	1	156331.25	2286.89	1

Table B- 13: Adjusted Production Capacity of Acetic Acid for the Structurally Integrated Plant Part 2

Component	Net Reaction Effluent/Production				Liquid Catalyst Solvent Ideal Feed				CO VENT (100%)			
	wt%	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*	*wt%*	$\mathcal{F}_{mass}$	$\mathcal{F}_{mole}$	*mol%*
Acetic Acid	1	61371.1	1022	1	0.4374	41538.30	691.73	0.5469	0	0	0	0
Water	0	0	0	0	0.0342	3251.48	180.44	0.1427	0	0	0	0
Carbon Monoxide	0	0	0	0	0	0	0	0	1	33187.81	1184.86	1
Methanol	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Acetate	0	0	0	0	0.0496	4714.65	63.64	0.0503	0	0	0	0
Dimethyl Ether	0	0	0	0	0	0	0	0	0	0	0	0
Methyl Iodide	0	0	0	0	0.2602	24711.26	174.10	0.1376	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Propionic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lithium Iodide	0	0	0	0	0.2185	20744.45	154.98	0.1225	0	0	0	0
TOTAL, if any	1	61371.1	1022	1	1	94960.15	1264.89	1	1	33187.81	1184.86	1

APPENDIX C

UNITS/EQUIPMENT OPERATING CONDITIONS

APPENDIX C.1 OPERATING CONDITIONS OF ACETIC ACID STANDALONE PLANT

Table C- 1: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Acetic Acid Plant Part 1

Heater Batch 1				
Name	E-103	E-104	E-105	E-113
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-5**	**-5**	**-3**	**-0.5**
Specified temperature [C]	**180**	**180**	**124.1**	**111**
Calculated pressure [bar]	29.207103	29.310524	1.29215728	0.9474194
Calculated temperature [C]	180	180	124.1	111
Calculated vapor fraction	0	0	1	1
Calculated heat duty [cal/sec]	355260.19	827036.42	-60307.289	287926.73
Net duty [cal/sec]	355260.19	827036.42	-60307.289	287926.73
First liquid / total liquid	1	1		

Table C- 2: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Acetic Acid Plant Part 2

Heater Batch 2				
Name	E-114	EX-101	EX-102	EX-103
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-1.5**	**-3**	**-5**	**-1.5**
Specified temperature [C]	**89.109411**	**180**	**210.7**	
Calculated pressure [bar]	1.3955785	29.793157	29.6552621	0.9098286
Calculated temperature [C]	89.109411	180	210.7	74.256955
Calculated vapor fraction	0	1	0	0
Calculated heat duty [cal/sec]	-1571083	4111.0412	563997.731	4814.2667
Net duty [cal/sec]	-1571083	4111.0412	563997.731	4814.2667
First liquid / total liquid	1		1	1

Table C- 3: Heat Exchange Equipment (Model: MHeatX) Operating Conditions and Specifications for Acetic Acid Plant

MHeatX			
Name	E106	E107	E108
Duty [cal/sec]	-12322.848	9908.6435	-367891.222

Table C- 4: Flash Separators (Model: Flash2) Operating Conditions and Specifications for Acetic Acid Plant

Flash2	
Name	VX-100
Property method	**NRTL-HOC**
Use true species approach for electrolytes	**YES**
Free-water phase properties method	**STEAM-TA**
Water solubility method	**3**
Pressure [bar]	**-0.001**
Outlet temperature [C]	131.316831
Outlet pressure [bar]	1.499
Vapor fraction	0.59970659

Table C- 5: Recycle and Ideal Separators (Model: Separators) Operating Conditions and Specifications for Acetic Acid Plant

Sep		
Name	RECYCLEX	RVX
Property method	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Heat duty [cal/sec]	191667.077	27827.2497

Table C- 6: Pumps Operating Conditions and Specifications for Acetic Acid Plant

Pump		
Name	PX-100	PX-101
Property method	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Specified discharge pressure [bar]	**30**	**30**
Fluid power [kW]	20.8228273	33.4956771
Calculated brake power [kW]	37.7160975	54.9875356
Electricity [kW]	37.7160975	54.9875356
Volumetric flow rate [l/min]	431.014045	690.865861
Calculated discharge pressure [bar]	30	30
Calculated pressure change [bar]	28.98675	29.0901714
Calculated pressure ratio		
NPSH available [m-kgf/kg]	10.8668173	0
NPSH required		
Head developed [m-kgf/kg]	372.776941	206.775863
Pump efficiency used	0.552093897	0.609150361
Net work required [kW]	37.7160975	54.9875356

Table C- 7: Compressors Operating Conditions and Specifications for Acetic Acid Plant

Compr	
Name	CX-100
Property method	**NRTL-HOC**
Use true species approach for electrolytes	**YES**
Free-water phase properties method	**STEAM-TA**
Water solubility method	**3**
Specified discharge pressure [bar]	**30**
Indicated horsepower [kW]	916.183614
Calculated brake horsepower [kW]	916.183614
Net work required [kW]	916.183614
Efficiency (polytropic / isentropic) used	0.72
Calculated discharge pressure [bar]	30
Calculated pressure change [bar]	20
Calculated pressure ratio	3
Outlet temperature [C]	177.249382
Isentropic outlet temperature [C]	135.912072
Vapor fraction	1
Head developed [m-kgf/kg]	11651.6983
Isentropic power requirement [kW]	659.652202
Inlet heat capacity ratio	1.42075639
Inlet volumetric flow rate [l/min]	30501.86
Outlet volumetric flow rate [l/min]	15551.4704
Inlet compressibility factor	0.995009446
Outlet compressibility factor	1.00746652

Table C- 8: Valves Operating Conditions and Specifications for Acetic Acid Plant

Valve	
Name	VLX-100
Property method	**NRTL-HOC**
Use true species approach for electrolytes	**YES**
Free-water phase properties method	**STEAM-TA**
Water solubility method	**3**
Specified outlet pressure [bar]	**1.5**
Calculation type	**ADIAB-FLASH**
Valve pressure specification (design mode)	**P-OUT**
Valve pressure specification (rating mode)	**VAL-POSN**
Calculated outlet pressure [bar]	1.5
Calculated pressure drop [bar]	28.1552621
Piping geometry factor	1

Table C- 9: Distillation Columns (Model: RadFrac) Operating Conditions and Specifications for Acetic Acid Plant

RadFrac	
Name	TX-100
Property method	**NRTL-HOC**
Use true species approach for electrolytes	**YES**
Free-water phase properties method	**STEAM-TA**
Water solubility method	**3**
Number of stages	**44**
Condenser	**TOTAL**
Reboiler	**KETTLE**
Number of phases	**2**
Free-water	**NO**
Top stage pressure [atm]	**1**
Specified reflux ratio	**2.25**
Specified bottoms rate [kmol/hr]	**637.5578**
Calculated molar reflux ratio	2.25
Calculated bottoms rate [kmol/hr]	637.5578
Calculated boilup rate [kmol/hr]	1079.86925
Calculated distillate rate [kmol/hr]	221.257409
Condenser / top stage temperature [C]	54.0613001
Condenser / top stage pressure [bar]	1.01325
Condenser / top stage heat duty [cal/sec]	-1635458.99
Condenser / top stage reflux rate [kmol/hr]	497.829169
Reboiler pressure [bar]	1.01325
Reboiler temperature [C]	117.798593
Reboiler heat duty [cal/sec]	1686852.01
Calculated molar boilup ratio	1.69375899
Calculated mass boilup ratio	1.68895289

Table C- 10: Reactors (Model: RStoic) Operating Conditions and Specifications for Acetic Acid Plant

RStoic	
Name	RX-100
Property method	**NRTL-HOC**
Use true species approach for electrolytes	**YES**
Free-water phase properties method	**STEAM-TA**
Water solubility method	**3**
Specified pressure [bar]	**30**
Specified temperature [C]	**180**
Outlet temperature [C]	180
Outlet pressure [bar]	30
Calculated heat duty [cal/sec]	-5674778.34
Net heat duty [cal/sec]	-5674778.34
Calculated vapor fraction	0.056665898
First liquid / total liquid	1

Table C- 11: Mixers Operating Conditions and Specifications for Acetic Acid Plant

Mixer		
Name	MAKEUPX	MIX100
Property method	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Outlet temperature [C]	21.472458	73.5821833
Calculated outlet pressure [bar]	1.01325	1.01325
Vapor fraction	0	0.062503811
First liquid /Total liquid	1	1

Table C- 12: Splitters Operating Conditions and Specifications for Acetic Acid Plant

FSplit	
Name	B4
Property method	**NRTL-HOC**
Use true species approach for electrolytes	**YES**
Free-water phase properties method	**STEAM-TA**
Water solubility method	**3**
First calculated split fraction	0.99
Second outlet stream	**0.01**
Second specified split fraction	**0.01**
Second calculated split fraction	0.01

APPENDIX C.2 OPERATING CONDITIONS OF ETHANOL STANDALONE PLANT

Table C- 13: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Ethanol Plant Part 1

Heater						
Name	C112	C115	C123	E-104	E-105	E-107
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-0.3**	**-3**	**-0.3**	**-3**	**-5**	**-5**
Specified temperature [C]	**78.15**	**93.33**	**3**	**170**	**180**	
Calculated pressure [bar]	39.5035775	24.5863146	39.4828932	39.7931573	39.6552621	0.655262135
Calculated temperature [C]	78.15	93.33	3	170	180	52.081507
Calculated vapor fraction	0.821349557	1	0.789291433	1	0	0
Calculated heat duty [cal/sec]	-756953.891	-27275.4145	-1090528.63	1653.78274	198332.591	12801.4117
Net duty [cal/sec]	-756953.891	-27275.4145	-1090528.63	1653.78274	198332.591	12801.4117
First liquid / total liquid	1		1		1	1

Table C- 14: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Ethanol Plant Part 2

Heater						
Name	E-300	H-111	H-114	H106	H107	H110
Property method	**SR-POLAR**	**SR-POLAR**	**SR-POLAR**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-1.5**	**-5**	**-5**	**-5**	**-5**	**-5**
Specified temperature [C]	**200**	**83.2**	**74.82**	**200**	**170**	**168.46**
Calculated pressure [bar]	39.8965786	39.3105243	39.6552621	38.9657864	39.3105243	39.3105243
Calculated temperature [C]	200	83.2	74.82	200	170	168.46
Calculated vapor fraction	1	0	0	0	0	0
Calculated heat duty [cal/sec]	298185.611	37619.7158	168649.514	192076.232	1117260.74	206122.593
Net duty [cal/sec]	298185.611	37619.7158	168649.514	192076.232	1117260.74	206122.593
First liquid / total liquid		1	1	1	1	1

Table C- 15: Heat Exchange Equipment (Model: MHeatX) Operating Conditions and Specifications for Ethanol Plant

MHeatX						
Name	I103	I104	I109	I112	I113	I116
Duty [cal/sec]	-498558.399	-61931.7499	-45217.0419	-409464.608	243042.676	591926.284

Table C- 16: Flash Separator (Model: Flash2) Operating Conditions and Specifications for Ethanol Plant

Flash2		
Name	V-100	V-300
Property method	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Pressure [bar]	**-0.001**	**-0.001**
Outlet temperature [C]	102.099847	0.257561141
Outlet pressure [bar]	1.499	24.999
Vapor fraction	0.36320742	0.790315677
First liquid / total liquid	1	1

Table C- 17: Recycle and Ideal Separator Equipment (Model: Separator) Operating Conditions and Specifications for Ethanol Plant

Sep		
Name	R100V	RECYCLE
Property method	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Heat duty [cal/sec]	-118887.666	9590.09554

Table C- 18: Pumps Operating Conditions and Specifications for Ethanol Plant

Pump					
Name	P-100	P-102	P-200	P-201	P-300
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**	**3**
Specified discharge pressure [bar]	**40**	**40**	**3.5**	**3.5**	**40**
Fluid power [kW]	29.57	96.79	0.81	0.42	39.17
Calculated brake power [kW]	52.91	140.33	1.74	1.23	66.03
Electricity [kW]	52.91	140.33	1.74	1.23	66.03
Volumetric flow rate [l/min]	455.14	1476.09	228.51	99.10	602.81
Calculated discharge pressure [bar]	40.00	40.00	3.55	3.55	40.00
Calculated pressure change [bar]	38.99	39.34	2.13	2.53	38.99
NPSH available [m-kgf/kg]	10.87	1.35	0.00	10.87	0.00
Head developed [m-kgf/kg]	501.38	389.05	24.50	32.58	533.30
Pump efficiency used	0.56	0.69	0.47	0.34	0.59
Net work required [kW]	52.91	140.33	1.74	1.23	66.03

Table C- 19: Compressors Operating Conditions and Specifications for Ethanol Plant

Compr				
Name	C-100	C-101	C-300	C-301
Property method	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified discharge pressure [bar]	**25**	**40**	**25**	**40**
Indicated horsepower [kW]	811.736046	499.836729	1717.38179	2014.25922
Calculated brake horsepower [kW]	811.736046	499.836729	1717.38179	2014.25922
Net work required [kW]	811.736046	499.836729	1717.38179	2014.25922
Power loss [kW]	0	0	0	0
Efficiency (polytropic / isentropic) used	0.72	0.72	0.72	0.72
Calculated discharge pressure [bar]	25	40	25	40
Calculated pressure change [bar]	15	15.4136854	10	15.2068427
Calculated pressure ratio	2.5	1.62692135	1.66666667	1.61334837
Outlet temperature [C]	148.675333	169.008592	73.1506065	154.903741
Isentropic outlet temperature [C]	115.02786	148.522358	55.6214398	134.516444
Vapor fraction	1	1	1	1
Head developed [m-kgf/kg]	9445.0735	5815.92338	64848.1691	76058.2319
Isentropic power requirement [kW]	584.449953	359.882445	1236.51489	1450.26664
Inlet heat capacity ratio	1.42075639	1.43053691	1.41154398	1.40285285
Inlet volumetric flow rate [l/min]	33338.229	16748.8522	89638.017	68280.8629
Outlet volumetric flow rate [l/min]	19050.236	12537.9749	65942.8839	51204.6164
Inlet compressibility factor	0.995009446	0.999879577	1.00957037	1.01382361
Outlet compressibility factor	1.00467872	1.00931984	1.01420331	1.01939181

Table C- 20: Valves Operating Conditions and Specifications for Ethanol Plant

Valve		
Name	VL-100	VL-300
Property method	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Specified outlet pressure [bar]	**1.5**	**25**
Calculation type	**ADIAB-FLASH**	**ADIAB-FLASH**
Valve pressure specification (design mode)	**P-OUT**	**P-OUT**
Valve pressure specification (rating mode)	**VAL-POSN**	**VAL-POSN**
Calculated outlet pressure [bar]	1.5	25
Calculated pressure drop [bar]	38.1552621	14.4828932
Piping geometry factor	1	1

Table C- 21: Distillation Columns (Model: RadFrac) Operating Conditions and Specifications for Ethanol Plant

RadFrac				
Name	T-100	T-200	T-300	T-301
Property method	**NRTL-HOC**	**SR-POLAR**	**SR-POLAR**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Number of stages	**26**	**42**	**40**	**41**
Condenser	**TOTAL**	**TOTAL**	**PARTIAL-V**	**PARTIAL-V**
Reboiler	**KETTLE**	**KETTLE**	**KETTLE**	**KETTLE**
Number of phases	**2**	**2**	**2**	**2**
Free-water	**NO**	**NO**	**NO**	**NO**
Top stage pressure [atm]	**1.4**	**1**	**1**	**1**
Specified reflux ratio	**2.3**	**3.4**	**6**	**3**
Specified bottoms rate [kmol/hr]	**359.1998**	**352.5615**		**338.2567**
Specified distillate rate [kmol/hr]			**95**	
Calculated molar reflux ratio	2.3	3.4	6	3
Calculated bottoms rate [kmol/hr]	359.20	352.56	404.33	338.26
Calculated boilup rate [kmol/hr]	290.40	23.03	627.04	1585.04
Calculated distillate rate [kmol/hr]	345.56	153.78	95.00	389.19
Condenser / top stage temperature [C]	58.53	55.24	43.22	63.78
Condenser / top stage pressure [bar]	1.42	1.01	1.01	1.01
Condenser / top stage heat duty [cal/sec]	-2302542.44	-1414404.38	-1144719.19	-2833659.35
Condenser / top stage reflux rate [kmol/hr]	794.78	522.84	570.00	1167.58
Reboiler pressure [bar]	1.42	1.01	1.01	1.01
Reboiler temperature [C]	112.05	97.57	55.13	77.78
Reboiler heat duty [cal/sec]	710270.37	63117.82	1313564.38	4143696.25
Calculated molar boilup ratio	0.81	0.07	1.55	4.69
Calculated mass boilup ratio	0.69	0.07	1.52	4.67

Table C- 22: Reactors (Model: RStoich) Operating Conditions and Specifications for Ethanol Plant

RStoic			
Name	R-100	R-200	R-300
Property method	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**
Specified pressure [bar]	**40**	**3.5**	**40**
Specified temperature [C]	**170**	**130**	**200**
Outlet temperature [C]	170	130	200
Outlet pressure [bar]	40	3.546375	40
Calculated heat duty [cal/sec]	-3421067.66	800578.671	-114870.715
Net heat duty [cal/sec]	-3421067.66	800578.671	-114870.715
Calculated vapor fraction	0.205960931	1	1
First liquid / total liquid	1		

Table C- 23: Mixers Operating Conditions and Specifications for Ethanol Plant Part 1

Mixer		
Name	B11	B17
Property method	**SR-POLAR**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Outlet temperature [C]	10.5878139	124.307691
Calculated outlet pressure [bar]	15	3.20163714
Vapor fraction	1	0.229372897
First liquid /Total liquid	1	1

Table C- 24: Mixers Operating Conditions and Specifications for Ethanol Plant Part 2

Mixer			
Name	M-300	MAKEUP	MIX100
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**
Outlet temperature [C]	50.7454355	25.0000257	40.3927843
Calculated outlet pressure [bar]	1.01325	1	1
Vapor fraction	0.028839693	0	0
First liquid /Total liquid	1	1	1

Table C- 25: Splitters Operating Conditions and Specifications for Ethanol Plant

FSplit		
Name	B4	B12
Property method	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
First calculated split fraction	0.99	0.015836912
Second outlet stream	**0.01**	
Second specified split fraction	**0.01**	
Second calculated split fraction	0.01	0.984163088

APPENDIX C.3 OPERATING CONDITIONS OF STRUCTURALLY INTEGRATED PLANT

Table C- 26: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Structurally Integrated Plant Part 1

Heater				
Name	C111	C115	C120	C129
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-1.5**	**-43.51132132**	**-0.3**	**-0.375**
Specified temperature [C]	**117.99**	**149.06**	**95.55**	**59.76**
Specified vapor fraction			**1**	
Calculated pressure [bar]	1.39557864	36.7931573	1.3542101	36.6121699
Calculated temperature [C]	117.99	149.06	95.55	59.76
Calculated vapor fraction	0.868871682	1	0.090755427	0.804137012
Calculated heat duty [cal/sec]	-500816.855	-258612.635	-1928590.84	-890445.747
Net duty [cal/sec]	-500816.855	-258612.635	-1928590.84	-890445.747
First liquid / total liquid	1		1	1

Table C- 27: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Structurally Integrated Plant Part 2

Heater				
Name	C132	E-200	E-300	E-301
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-0.375**	**-5**	**-3**	**-2.175566066**
Specified temperature [C]	**3**	**130**	**200**	**82.22222222**
Specified vapor fraction				
Calculated pressure [bar]	36.5863146	3.20163714	39.7931573	24.85
Calculated temperature [C]	3	130	200	82.2222222
Calculated vapor fraction	0.788149179	0	1	1
Calculated heat duty [cal/sec]	-756085.8	40986.6402	307725.765	58622.51
Net duty [cal/sec]	-756085.8	40986.6402	307725.765	58622.51
First liquid / total liquid	1	1		

Table C- 28: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Structurally Integrated Plant Part 3

Heater				
Name	EX-101	EX-102	H108	H109
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-3**	**-5**	**-5**	**-3**
Specified temperature [C]	**180**	**210.7**	**200**	**130**
Specified vapor fraction				**0**
Calculated pressure [bar]	29.7931573	29.6552621	39.3105243	2.68453034
Calculated temperature [C]	180	210.7	200	130
Calculated vapor fraction	1	0	0	1
Calculated heat duty [cal/sec]	6423.50191	881246.454	404899.215	35454.4891
Net duty [cal/sec]	6423.50191	881246.454	404899.215	35454.4891
First liquid / total liquid		1	1	

Table C- 29: Heat Exchange Equipment (Model: Heater) Operating Conditions and Specifications for Structurally Integrated Plant Part 4

Heater				
Name	H110	H117	H119	H131
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**
Specified pressure [psi]	**-5**	**-5**	**-0.75**	**-5**
Specified temperature [C]	**180**	**157.02**	**100.2**	**120.99**
Specified vapor fraction				
Calculated pressure [bar]	29.3105243	29.3105243	3.09821578	39.6552621
Calculated temperature [C]	180	157.02	100.2	120.99
Calculated vapor fraction	0	0	1	0
Calculated heat duty [cal/sec]	634842.574	355383.892	784390.874	246166.722
Net duty [cal/sec]	634842.574	355383.892	784390.874	246166.722
First liquid / total liquid	1	1		times

Table C- 30: Heat Exchange Equipment (Model: MHeatX) Operating Conditions and Specifications for Structurally Integrated Plant Part 1

MHeatX							
Name	I107	I112	I116	I118	I121	I122	I125
Duty [cal/sec]	-222900.508	-19647.1159	799879.341	-572189.142	152839.314	-97041.1717	104496.841

Table C- 31: Heat Exchange Equipment (Model: MHeatX) Operating Conditions and Specifications for Structurally Integrated Plant Part 2

MHeatX				
Name	I118	I121	I122	I125
Duty [cal/sec]	-572189.142	152839.314	-97041.1717	104496.841

Table C- 32: Separator (Model: Flash2) Operating Conditions and Specifications for Structurally Integrated Plant

Flash2		
Name	V-100	V-300
Property method	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Pressure [bar]	**-0.001**	**-0.001**
Outlet temperature [C]	131.316829	0.338466023
Outlet pressure [bar]	1.499	24.999
Vapor fraction	0.599706538	0.7890647
First liquid / total liquid	1	1

Table C- 33: Recycle and Separator (Model: Separator) Operating Conditions and Specifications for Structurally Integrated Plant

Sep		
Name	RECYCLEX	RVX
Property method	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Heat duty [cal/sec]	-5116.38716	43479.1546

Table C- 34: Pumps Operating Conditions for Structurally Integrated Plant

Pump					
Name	B2	P-200	P-201	P-300	PX-101
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**	**3**
Specified discharge pressure [bar]	**30**	**3.5**	**3.5**	**40**	**30**
Fluid power [kW]	32.54	1.60	1.12	33.08	52.28
Calculated brake power [kW]	53.67	2.98	2.29	57.75	79.54
Electricity [kW]	53.67	2.98	2.29	57.75	79.54
Volumetric flow rate [l/min]	673.46	377.96	264.14	509.09	1069.34
Calculated discharge pressure [bar]	30.00	3.55	3.55	40.00	30.00
Calculated pressure change [bar]	28.99	2.53	2.53	38.99	29.33
NPSH available [m-kgf/kg]	10.87	0.00	10.87	-0.03	0.00
Head developed [m-kgf/kg]	372.78	27.33	32.58	447.81	206.53
Pump efficiency used	0.61	0.54	0.49	0.57	0.66
Net work required [kW]	53.67	2.98	2.29	57.75	79.54

Table C- 35: Compressor Operating Conditions and Specifications for Structurally Integrated Plant

Compr			
Name	C-300	C-301	CX-100
Property method	**SR-POLAR**	**SR-POLAR**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**
Specified discharge pressure [bar]	**25**	**40**	**30**
Indicated horsepower [kW]	1717.97568	2001.84525	1431.5369
Calculated brake horsepower [kW]	1717.97568	2001.84525	1431.5369
Net work required [kW]	1717.97568	2001.84525	1431.5369
Power loss [kW]	0	0	0
Efficiency (polytropic / isentropic) used	0.72	0.72	0.72
Calculated discharge pressure [bar]	25	40	30
Calculated pressure change [bar]	10	15.15	20
Calculated pressure ratio	1.66666667	1.60965795	3
Outlet temperature [C]	73.2839401	154.089796	177.249382
Isentropic outlet temperature [C]	55.7483453	133.826833	135.912072
Vapor fraction	1	1	1
Head developed [m-kgf/kg]	64872.727	75591.9669	11651.6983
Isentropic power requirement [kW]	1236.94249	1441.32858	1030.70657
Inlet heat capacity ratio	1.41152366	1.40289601	1.42075639
Inlet volumetric flow rate [l/min]	89669.2886	68053.4442	47659.1563
Outlet volumetric flow rate [l/min]	65965.4287	51106.7558	24299.1726
Inlet compressibility factor	1.00956832	1.01386556	0.995009446
Outlet compressibility factor	1.0141994	1.01942197	1.00746652

Table C- 36: Valves Operating Conditions for Structurally Integrated Plant

Valve		
Name	VL-300	VLX-100
Property method	**SR-POLAR**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**
Specified outlet pressure [bar]	**25**	**1.5**
Calculation type	**ADIAB-FLASH**	**ADIAB-FLASH**
Valve pressure specification (design mode)	**P-OUT**	**P-OUT**
Valve pressure specification (rating mode)	**VAL-POSN**	**VAL-POSN**
Calculated outlet pressure [bar]	25	1.5
Calculated pressure drop [bar]	11.5863146	28.1552621
Piping geometry factor	1	1

Table C- 37: Distillation Columns (Model: RadFrac) Operating Conditions and Specifications for Structurally Integrated Plant

RadFrac			
Name	T-100	T-200	T-300
Property method	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**
Number of stages	**43**	**40**	**41**
Condenser	**TOTAL**	**TOTAL**	**PARTIAL-V**
Reboiler	**KETTLE**	**KETTLE**	**KETTLE**
Number of phases	**2**	**2**	**2**
Free-water	**NO**	**NO**	**NO**
Top stage pressure [atm]	**1**	**1**	**1**
Specified reflux ratio	**2.23**	**2**	**3**
Specified bottoms rate [kmol/hr]	**996.1816**		**338.257**
Specified distillate rate [kmol/hr]		**410**	
Calculated molar reflux ratio	2.23	2	3
Calculated bottoms rate [kmol/hr]	996.1816	340.37424	338.257
Calculated boilup rate [kmol/hr]	1635.10483	218.799495	1605.76599
Calculated distillate rate [kmol/hr]	345.717045	410	394.723311
Condenser / top stage temperature [C]	54.1042176	54.9203214	63.7924025
Condenser / top stage pressure [bar]	1.01325	1.01325	1.01325
Condenser / top stage heat duty [cal/sec]	-2536252.76	-2547881.24	-2874090.99
Condenser / top stage subcooled duty			
Condenser / top stage reflux rate [kmol/hr]	770.949011	820	1184.16993
Condenser / top stage free water reflux ratio			
Reboiler pressure [bar]	1.01325	1.01325	1.01325
Reboiler temperature [C]	117.751079	100.500708	77.8449222
Reboiler heat duty [cal/sec]	2558368.58	588508.055	4199649.49
Basis for specified distillate to feed ratio	**MOLE**	**MOLE**	**MOLE**
Basis for specified bottoms to feed ratio	**MOLE**	**MOLE**	**MOLE**
Basis for specified boilup ratio	**MOLE**	**MOLE**	**MOLE**
Calculated molar boilup ratio	1.64137224	0.642820371	4.7471774
Calculated mass boilup ratio	1.6356576	0.622761104	4.73126294

Table C- 38: Reactor (Model: RStoic) Operating Conditions and Specifications for Structurally Integrated Plant

RStoic			
Name	R-100	R-200	R-300
Property method	**NRTL-HOC**	**NRTL-HOC**	**SR-POLAR**
Use true species approach for electrolytes	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**
Specified pressure [bar]	**30**	**3.5**	**40**
Specified temperature [C]	**180**	**130**	**200**
Outlet temperature [C]	180	130	200
Outlet pressure [bar]	30	3.546375	40
Calculated heat duty [cal/sec]	-8866878.93	610305.625	-109914.48
Net heat duty [cal/sec]	-8866878.93	610305.625	-109914.48
Calculated vapor fraction	0.056666193	1	1
First liquid / total liquid	1		

Table C- 39: Mixer Operating Conditions and Specifications for Structurally Integrated Plant

Mixer					
Name	B1	B11	B17	MAKEUPX	MIX100
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Henry's component list ID					
Electrolyte chemistry ID					
Use true species approach for electrolytes	**YES**	**YES**	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**	**3**	**3**
Specified pressure [bar]	**0**	**0**	**0**	**0**	**0**
Temperature estimate [C]					
EO Model components					
Outlet temperature [C]	118.143192	10.4578768	125.07115	24.8957435	53.986965
Calculated outlet pressure [bar]	28.9657864	15	2.68453034	1.01325	1.01325
Vapor fraction	0.691294051	1	0.560802103	0	0
First liquid /Total liquid	1	1	1	1	1

Table C- 40: Splitter Operating Conditions for Structurally Integrated Plant

FSplit			
Name	B4	B9	B12
Property method	**NRTL-HOC**	**NRTL-HOC**	**NRTL-HOC**
Use true species approach for electrolytes	**YES**	**YES**	**YES**
Free-water phase properties method	**STEAM-TA**	**STEAM-TA**	**STEAM-TA**
Water solubility method	**3**	**3**	**3**
First calculated split fraction	0.99	0.640445477	0.015909276
Second outlet stream	**0.01**		
Second specified split fraction	**0.01**		
Second calculated split fraction	0.01	0.359554523	0.984090724

APPENDIX D

STREAMS DATA OF SIMULATED PLANTS

APPENDIX D.1 STREAMS DATA OF ACETIC ACID STANDALONE PLANT

Table D- 1: Streams Data for Acetic Acid Standalone Plant Part 1

Stream	ACOH	ACOHX	BLEEDX	COX	H2O	INTR-100
Destination		MAKEUPX		CX-100	MAKEUPX	RVX
Source	TX-100		RECYCLEX			RX-100
	LIQUID	LIQUID	MIXED	VAPOR	LIQUID	MIXED
ACETI-01	0.9987306	1	0.0217201	0	0	0.6396159
WATER	1.27E-03	0	0.0799702	0	1	0.0202036
CO2	0	0	0	0	0	0
CO	0	0	0	1	0	0.0283611
METHA-01	0	0	0	0	0	0
ACETATE	3.64E-13	0	0.1364079	0	0	0.0293028
DIMET-01	0	0	0	0	0	0
IODIDE	1.59E-24	0	0.758113	0	0	0.1535875
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	3.79E-03	0	0	0.128929
Total Flow kmol/hr	637.5578	6	224.6666	741.9733	86	1534.075
Total Flow kg/hr	38173.91	360.3154	18704.3	20782.97	1549.314	1.01E+05
Total Flow l/min	673.1767	5.599183	75682.43	30501.86	25.97889	3255.693
Temperature C	117.7986	25	73.58218	25	25	180
Pressure bar	1.01325	1.01325	1.01325	10	1.01325	30
Vapor Frac	0	0	0.7256445	1	0	0.0566659
Liquid Frac	1	1	0.2743555	0	1	0.9433341
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-1.12E+05	-1.15E+05	-40167.7	-26418.64	-68275.29	-89894.53
Enthalpy cal/gm	-1877.757	-1921.717	-482.4741	-943.1727	-3789.854	-1368.718
Enthalpy cal/sec	-1.99E+07	-1.92E+05	-2.51E+06	-5.45E+06	-1.63E+06	-3.83E+07
Entropy cal/mol-K	-67.77444	-76.05761	-19.95319	16.72483	-39.00528	-44.79008
Entropy cal/gm-K	-1.131928	-1.266517	-0.2396676	0.5970934	-2.165122	-0.6819658
Density mol/cc	0.0157848	0.0178597	4.95E-05	4.05E-04	0.055173	7.85E-03
Density gm/cc	0.9451186	1.072524	4.12E-03	0.0113561	0.993957	0.515788
Average MW	59.87521	60.05256	83.25358	28.0104	18.01528	65.67789
Liq Vol 60F l/min	610.5999	5.763	182.0469	662.3077	25.87167	1384.491

Table D- 2: Streams Data for Acetic Acid Standalone Plant Part 2

Stream	LII	MEI	MEOAC	MEOHX	S4	S13
Destination	MAKEUPX	MAKEUPX	MAKEUPX	PX-100		EX-102
Source					B4	RVX
	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
ACETI-01	0	0	0	0	0.6288452	0.6582856
WATER	0	0	0	0	0.0122764	0.0207934
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0	0	0	1	0	0
ACETATE	0	0	1	0	0.0104785	0.0301581
DIMET-01	0	0	0	0	0	0
IODIDE	0	1	0	0	0.0337969	0.1580706
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	1	0	0	0	0.3146029	0.1326923
Total Flow kmol/hr	1.5	100	34.5	639.9569	5.732438	1432.059
Total Flow kg/hr	200.7682	14193.93	2555.741	20505.6	412.9083	97897.32
Total Flow l/min	0.9679924	116.6347	45.73592	431.014	5.132661	1491.607
Temperature C	25	25	25	25	131.3168	180
Pressure bar	1.01325	1.01325	1.01325	1.01325	1.499	30
Vapor Frac	0	0	0	0	0	0
Liquid Frac	1	1	1	1	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-69517.37	-3284.064	-1.06E+05	-57034.64	-1.00E+05	-94423.5
Enthalpy cal/gm	-519.3853	-23.1371	-1433.185	-1779.988	-1392.744	-1381.243
Enthalpy cal/sec	-28965.57	-91224.01	-1.02E+06	-1.01E+07	-1.60E+05	-3.76E+07
Entropy cal/mol-K	-5.82161	-22.64957	-93.83548	-57.66153	-51.36059	-49.15289
Entropy cal/gm-K	-0.043495	-0.1595723	-1.266687	-1.799552	-0.713043	-0.719017
Density mol/cc	0.0258266	0.0142896	0.0125721	0.0247461	0.0186142	0.0160013
Density gm/cc	3.45678	2.028261	0.9313397	0.7929208	1.340787	1.093869
Average MW	133.8455	141.9393	74.07944	32.04216	72.03015	68.36124
Liq Vol 60F l/min	0.953925	104.5167	45.89828	430.2067	5.035333	1293.428

Table D- 3: Streams Data for Acetic Acid Standalone Plant Part 3

Stream	SI1-100	SI1-109	SI1-115	SI2-100	SI2-115	SI3-115
Destination	E106	E-104	E106	E-103	E107	E108
Source	E108	E107	E-105	E106	E106	E107
	LIQUID	LIQUID	VAPOR	LIQUID	VAPOR	VAPOR
ACETI-01	0	0.4374472	0.6797606	0	0.6797606	0.6797606
WATER	0	0.0342315	0.027006	0	0.027006	0.027006
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	1	0	0	1	0	0
ACETATE	0	0.0496483	0.0445131	0	0.0445131	0.0445131
DIMET-01	0	0	0	0	0	0
IODIDE	0	0.2602262	0.2487203	0	0.2487203	0.2487203
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0.2184468	6.60E-19	0	6.60E-19	6.60E-19
Total Flow kmol/hr	639.9569	792.1021	858.8152	639.9569	858.8152	858.8152
Total Flow kg/hr	20505.6	59466.28	56606.49	20505.6	56606.49	56606.49
Total Flow l/min	506.632	692.3368	2.72E+05	509.4639	2.85E+05	3.41E+05
Temperature C	114.796	76.77957	124.1	117.3	122.2664	118.7531
Pressure bar	29.89658	29.65526	1.292157	29.55184	1.22321	1.016367
Vapor Frac	0	0	1	0	1	1
Liquid Frac	1	1	0	1	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-54914.44	-85638.08	-88376.58	-54845.12	-88428.23	-88469.77
Enthalpy cal/gm	-1713.818	-1140.716	-1340.821	-1711.655	-1341.604	-1342.234
Enthalpy cal/sec	-9.76E+06	-1.88E+07	-2.11E+07	-9.75E+06	-2.11E+07	-2.11E+07
Entropy cal/mol-K	-51.6688	-48.78157	-41.08331	-51.49348	-41.13281	-40.96523
Entropy cal/gm-K	-1.612525	-0.6497799	-0.6233025	-1.607054	-0.6240536	-0.6215111
Density mol/cc	0.0210526	0.0190683	5.27E-05	0.0209356	5.02E-05	4.20E-05
Density gm/cc	0.6745725	1.431535	3.47E-03	0.6708229	3.31E-03	2.77E-03
Average MW	32.04216	75.074	65.91231	32.04216	65.91231	65.91231
Liq Vol 60F l/min	430.2067	678.7491	789.8943	430.2067	789.8943	789.8943

Table D- 4: Streams Data for Acetic Acid Standalone Plant Part 4

Stream	SI4-115	SI5-115	SX-100	SX-101	SX-102	SX-103
Destination	E-113	E-114	E108	RX-100	EX-101	RX-100
Source	E108	E-113	PX-100	E-103	CX-100	EX-101
	MIXED	VAPOR	LIQUID	LIQUID	VAPOR	VAPOR
ACETI-01	0.6797606	0.6797606	0	0	0	0
WATER	0.027006	0.027006	0	0	0	0
CO2	0	0	0	0	0	0
CO	0	0	0	0	1	1
METHA-01	0	0	1	1	0	0
ACETATE	0.0445131	0.0445131	0	0	0	0
DIMET-01	0	0	0	0	0	0
IODIDE	0.2487203	0.2487203	0	0	0	0
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	6.60E-19	6.60E-19	0	0	0	0
Total Flow kmol/hr	858.8152	858.8152	639.9569	639.9569	741.9733	741.9733
Total Flow kg/hr	56606.49	56606.49	20505.6	20505.6	20782.97	20782.97
Total Flow l/min	2.80E+05	3.52E+05	432.1095	608.9118	15551.47	15756.59
Temperature C	106.2084	111	26.68791	180	177.2494	180
Pressure bar	0.9818932	0.9474194	30	29.2071	30	29.79316
Vapor Frac	0.8319973	1	0	0	1	1
Liquid Frac	0.1680027	0	1	1	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-90011.9	-88804.97	-56983.97	-52846.65	-25356.91	-25336.97
Enthalpy cal/gm	-1365.631	-1347.32	-1778.406	-1649.285	-905.2678	-904.5557
Enthalpy cal/sec	-2.15E+07	-2.12E+07	-1.01E+07	-9.39E+06	-5.23E+06	-5.22E+06
Entropy cal/mol-K	-44.95017	-41.7264	-57.58844	-46.90976	17.41715	17.47514
Entropy cal/gm-K	-0.6819693	-0.6330594	-1.797271	-1.464001	0.6218101	0.6238805
Density mol/cc	5.12E-05	4.07E-05	0.0246834	0.0175164	7.95E-04	7.85E-04
Density gm/cc	3.37E-03	2.68E-03	0.7909106	0.5612636	0.0222733	0.0219833
Average MW	65.91231	65.91231	32.04216	32.04216	28.0104	28.0104
Liq Vol 60F l/min	789.8943	789.8943	430.2067	430.2067	662.3077	662.3077

Table D- 5: Streams Data for Acetic Acid Standalone Plant Part 5

Stream	SX-104	SX-105	SX-106	SX-107	SX-108	SX-109
Destination	MIX100	MIX100	RECYCLEX	EX-103	PX-101	E107
Source	MAKEUPX	B4	MIX100	RECYCLEX	EX-103	PX-101
	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	LIQUID
ACETI-01	0.0191046	0.6288452	0.3379739	0.4374472	0.4374472	0.4374472
WATER	0.0821478	0.0122764	0.0451756	0.0342315	0.0342315	0.0342315
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0	0	0	0	0	0
ACETATE	0.1355107	0.0104785	0.0704077	0.0496483	0.0496483	0.0496483
DIMET-01	0	0	0	0	0	0
IODIDE	0.7525916	0.0337969	0.3793583	0.2602262	0.2602262	0.2602262
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0.0106451	0.3146029	0.1670844	0.2184468	0.2184468	0.2184468
Total Flow kmol/hr	228	567.5113	1016.769	792.1021	792.1021	792.1021
Total Flow kg/hr	18860.07	40877.93	78170.58	59466.28	59466.28	59466.28
Total Flow l/min	187.0485	508.1335	29219.92	690.474	690.8659	691.5256
Temperature C	21.47246	131.3168	73.58218	73.58218	74.25696	75.3904
Pressure bar	1.01325	1.499	1.01325	1.01325	0.9098286	30
Vapor Frac	0	0	0.0625038	0	0	0
Liquid Frac	1	1	0.9374962	1	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-46752.77	-1.00E+05	-76368.13	-85764.68	-85742.8	-85683.11
Enthalpy cal/gm	-565.1958	-1392.744	-993.3242	-1142.402	-1142.11	-1141.315
Enthalpy cal/sec	-2.96E+06	-1.58E+07	-2.16E+07	-1.89E+07	-1.89E+07	-1.89E+07
Entropy cal/mol-K	-39.05066	-51.36059	-44.4269	-49.04521	-48.98034	-48.91462
Entropy cal/gm-K	-0.4720848	-0.713043	-0.577863	-0.6532915	-0.6524275	-0.6515521
Density mol/cc	0.0203155	0.0186142	5.80E-04	0.0191197	0.0191089	0.0190906
Density gm/cc	1.680497	1.340787	0.0445874	1.435397	1.434583	1.433215
Average MW	82.71959	72.03015	76.88137	75.074	75.074	75.074
Liq Vol 60F l/min	183.0035	498.498	860.796	678.7491	678.7491	678.7491

Table D- 6: Streams Data for Acetic Acid Standalone Plant Part 6

Stream	SX-110	SX-112	SX-113	SX-114	SX-115	SX-116
Destination	RX-100	VLX-100	VX-100	B4	E-105	TX-100
Source	E-104	EX-102	VLX-100	VX-100	VX-100	E-114
	LIQUID	LIQUID	MIXED	LIQUID	VAPOR	LIQUID
ACETI-01	0.4374472	0.6582856	0.6582856	0.6288452	0.6797606	0.6797606
WATER	0.0342315	0.0207934	0.0207934	0.0122764	0.027006	0.027006
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0	0	0	0	0	0
ACETATE	0.0496483	0.0301581	0.0301581	0.0104785	0.0445131	0.0445131
DIMET-01	0	0	0	0	0	0
IODIDE	0.2602262	0.1580706	0.1580706	0.0337969	0.2487203	0.2487203
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0.2184468	0.1326923	0.1326923	0.3146029	6.60E-19	6.60E-19
Total Flow kmol/hr	792.1021	1432.059	1432.059	573.2438	858.8152	858.8152
Total Flow kg/hr	59466.28	97897.32	97897.32	41290.83	56606.49	56606.49
Total Flow l/min	762.2912	1557.993	2.42E+05	513.2661	2.41E+05	862.9879
Temperature C	180	210.7	131.3373	131.3168	131.3168	89.10941
Pressure bar	29.31052	29.65526	1.5	1.499	1.499	1.395579
Vapor Frac	0	0	0.599605	0	1	0
Liquid Frac	1	1	0.400395	1	0	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-81879.43	-93005.68	-93005.68	-1.00E+05	-88123.78	-95390.67
Enthalpy cal/gm	-1090.65	-1360.503	-1360.503	-1392.744	-1336.985	-1447.236
Enthalpy cal/sec	-1.80E+07	-3.70E+07	-3.70E+07	-1.60E+07	-2.10E+07	-2.28E+07
Entropy cal/mol-K	-39.41638	-46.24949	-44.9518	-51.36059	-40.67305	-59.47895
Entropy cal/gm-K	-0.5250336	-0.6765455	-0.6575627	-0.713043	-0.6170782	-0.9023953
Density mol/cc	0.0173184	0.0153194	9.87E-05	0.0186142	5.93E-05	0.016586
Density gm/cc	1.300165	1.047259	6.75E-03	1.340787	3.91E-03	1.093227
Average MW	75.074	68.36124	68.36124	72.03015	65.91231	65.91231
Liq Vol 60F l/min	678.7491	1293.428	1293.428	503.5333	789.8943	789.8943

Table D- 7: Streams Data for Acetic Acid Standalone Plant Part 7

Stream	SX-117	VENT
Destination	MIX100	
Source	TX-100	RVX
	LIQUID	VAPOR
Mass Frac		
ACETI-01	0.0191732	0
WATER	0.0803066	0
CO2	0	0
CO	0	1
METHA-01	0	0
ACETATE	0.1366998	0
DIMET-01	0	0
IODIDE	0.7638202	0
HYDRO-01	0	0
ETHAN-01	0	0
PROPI-01	0	0
LITHI-01	0	0
Total Flow kmol/hr	221.2574	102.0165
Total Flow kg/hr	18432.58	2857.522
Total Flow l/min	192.2307	2151.604
Temperature C	54.0613	180
Pressure bar	1.01325	30
Vapor Frac	0	1
Liquid Frac	1	0
Solid Frac	0	0
Enthalpy cal/mol	-45452.01	-25337.12
Enthalpy cal/gm	-545.5878	-904.561
Enthalpy cal/sec	-2.79E+06	-7.18E+05
Entropy cal/mol-K	-36.83618	17.46097
Entropy cal/gm-K	-0.4421669	0.6233744
Density mol/cc	0.0191833	7.90E-04
Density gm/cc	1.59813	0.0221348
Average MW	83.30833	28.0104
Liq Vol 60F l/min	179.2945	91.06297

APPENDIX D.2 SREAMS DATA OF ETHANOL STANDALONE PLANT

Table D- 8: Stream data for Ethanol standalone plant Part 1

Stream	3-S10	74-S100	78-S10	82-S6	83-S100	93-S102
Destination	VL-300	H-111	C123	C-301	I103	C-101
Source	C123	H-114	C112	I104	H-111	C115
	MIXED	LIQUID	MIXED	VAPOR	LIQUID	VAPOR
Substream: MIXED						
Mass Frac						
ACETI-01	0	0	0	0	0	0
WATER	8.72E-03	0	8.72E-03	7.63E-05	0	0
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	1
METHA-01	0.3530759	1	0.3530759	0.0118304	1	0
ACETATE	0.0370092	0	0.0370092	7.62E-03	0	0
DIMET-01	0	0	0	0	0	0
IODIDE	9.94E-05	0	9.94E-05	6.81E-05	0	0
HYDRO-01	0.1625353	0	0.1625353	0.9742883	0	0
ETHAN-01	0.4385567	0	0.4385567	6.12E-03	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	3469.256	675.772	3469.256	3387.3	675.772	810.9695
Total Flow kg/hr	33962.17	21653.19	33962.17	6999.765	21653.19	22715.58
Total Flow l/min	28074.92	644.4591	36674.58	68596.46	652.8726	16748.85
Temperature C	3	74.82	78.15	82.22	83.2	93.33
Pressure bar	39.48289	39.65526	39.50358	24.79316	39.31052	24.58631
Vapor Frac	0.7892914	0	0.8213496	1	0	1
Liquid Frac	0.2107086	1	0.1786504	0	1	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-13446.29	-56068.89	-12314.66	331.9201	-55868.48	-25953.99
Enthalpy cal/gm	-1373.547	-1749.847	-1257.95	160.6215	-1743.593	-926.584
Enthalpy cal/sec	-1.30E+07	-1.05E+07	-1.19E+07	3.12E+05	-1.05E+07	-5.85E+06
Entropy cal/mol-K	-20.99822	-54.90992	-17.41656	-5.179054	-54.33948	16.34705
Entropy cal/gm-K	-2.144982	-1.713677	-1.779112	-2.506229	-1.695874	0.5836065
Density mol/cc	2.06E-03	0.0174764	1.58E-03	8.23E-04	0.0172512	8.07E-04
Density gm/cc	0.0201616	0.5599837	0.015434	1.70E-03	0.5527672	0.0226041
Average MW	9.789466	32.04216	9.789466	2.066473	32.04216	28.0104
Liq Vol 60F l/min	3036.852	454.2832	3036.852	3023.406	454.2832	723.8957

Table D- 9: Streams Data for Ethanol Standalone Plant Part 2

Stream	106-S10	112-S113	119-S10	121-S1	122-S102	125-S10
Destination	C112	H107	I116	H110	C115	I113
Source	I116	I116	I113	I113	I104	I112
	MIXED	LIQUID	MIXED	LIQUID	VAPOR	MIXED
Substream: MIXED						
Mass Frac						
ACETI-01	0	0.3812415	0	0	0	0
WATER	8.72E-03	0.0782071	8.72E-03	0.0109682	0	8.72E-03
CO2	0	0	0	0	0	0
CO	0	0	0	0	1	0
METHA-01	0.3530759	0.2528221	0.3530759	0.0585659	0	0.3530798
ACETATE	0.0370092	0.0937576	0.0370092	0.9303584	0	0.0370087
DIMET-01	0	0	0	0	0	0
IODIDE	9.94E-05	0.1165571	9.94E-05	1.07E-04	0	9.94E-05
HYDRO-01	0.1625353	0	0.1625353	0	0	0.1625375
ETHAN-01	0.4385567	0	0.4385567	0	0	0.4385512
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0.0774146	0	0	0	0
Total Flow kmol/hr	3469.256	1940.368	3469.256	404.3315	810.9695	3469.263
Total Flow kg/hr	33962.17	91332.46	33962.17	26962.1	22715.58	33961.87
Total Flow l/min	41775.65	1546.602	45675.59	574.8435	17407.26	47265.57
Temperature C	106.16	108.0627	121	121.685	110.2584	125.9753
Pressure bar	39.52426	39.65526	39.54495	39.65526	24.79316	39.56563
Vapor Frac	0.8789527	0	0.9382425	0	1	0.9653448
Liquid Frac	0.1210473	1	0.0617574	1	0	0.0346552
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-11529.18	-75656.3	-10914.95	-95242.22	-25832.91	-10662.61
Enthalpy cal/gm	-1177.713	-1607.327	-1114.969	-1428.28	-922.2613	-1089.204
Enthalpy cal/sec	-1.11E+07	-4.08E+07	-1.05E+07	-1.07E+07	-5.82E+06	-1.03E+07
Entropy cal/mol-K	-15.27174	-49.47754	-13.68583	-76.80176	16.65338	-13.05099
Entropy cal/gm-K	-1.560018	-1.051156	-1.398016	-1.151742	0.5945428	-1.333182
Density mol/cc	1.38E-03	0.02091	1.27E-03	0.0117229	7.76E-04	1.22E-03
Density gm/cc	0.0135494	0.9842271	0.0123925	0.7817229	0.0217491	0.0119755
Average MW	9.789466	47.06965	9.789466	66.68315	28.0104	9.78936
Liq Vol 60F l/min	3036.852	1426.406	3036.852	488.5767	723.8957	3036.858

Table D- 10: Streams Data for Ethanol Standalone Plant Part 3

Stream	130-S202	130-S203	143-S10	148-S10	168-S1	170-S100
Destination	B17	B17	I112	I109	H106	RECYCLE
Source	I109	I112	I109	I103	H110	I103
	LIQUID	VAPOR	VAPOR	VAPOR	LIQUID	LIQUID
Substream: MIXED						
Mass Frac						
ACETI-01	0.6614495	0	0	0	0	0
WATER	0.3294157	0	8.72E-03	8.72E-03	0.0109682	0
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	8.85E-03	1	0.3530798	0.3530798	0.0585659	1
ACETATE	6.35E-06	0	0.0370087	0.0370087	0.9303584	0
DIMET-01	0	0	0	0	0	0
IODIDE	2.74E-04	0	9.94E-05	9.94E-05	1.07E-04	0
HYDRO-01	0	0	0.1625375	0.1625375	0	0
ETHAN-01	0	0	0.4385512	0.4385512	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	359.1998	147.1369	3469.263	3469.263	404.3315	675.772
Total Flow kg/hr	12144.07	4714.583	33961.87	33961.87	26962.1	21653.19
Total Flow l/min	234.7858	22741.44	50787.25	51150.62	653.3437	620.586
Temperature C	130	130	143.0393	147.7347	168.46	170
Pressure bar	3.201637	3.442954	39.58631	39.79316	39.31052	38.96579
Vapor Frac	0	1	1	1	0	0
Liquid Frac	1	0	0	0	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-83206.89	-47009.08	-10237.71	-10190.79	-93406.99	-53212.54
Enthalpy cal/gm	-2461.11	-1467.101	-1045.8	-1041.007	-1400.758	-1660.704
Enthalpy cal/sec	-8.30E+06	-1.92E+06	-9.87E+06	-9.82E+06	-1.05E+07	-9.99E+06
Entropy cal/mol-K	-44.77935	-30.37365	-12.00083	-11.89912	-72.41391	-47.72307
Entropy cal/gm-K	-1.324493	-0.9479276	-1.225905	-1.215516	-1.08594	-1.489384
Density mol/cc	0.0254984	1.08E-04	1.14E-03	1.13E-03	0.0103144	0.0181487
Density gm/cc	0.8620673	3.46E-03	0.0111451	0.0110659	0.6877978	0.5815255
Average MW	33.80868	32.04216	9.78936	9.78936	66.68315	32.04216
Liq Vol 60F l/min	197.5618	98.91179	3036.858	3036.858	488.5767	454.2832

Table D- 11: Streams Data for Ethanol Standalone Plant Part 4

Stream	170-S113	200-S1	ACOH	BLEED100	CO	ETOH
Destination	R-100	R-300	MAKEUP		C-100	
Source	H107	H106		RECYCLE		T-301
	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID
Substream: MIXED						
Mass Frac						
ACETI-01	0.3812415	0	1	1.37E-04	0	0
WATER	0.0782071	0.0109682	0	7.09E-05	0	0.0196355
CO2	0	0	0	0	0	0
CO	0	0	0	0	1	0
METHA-01	0.2528221	0.0585659	0	8.76E-03	0	9.37E-03
ACETATE	0.0937576	0.9303584	0	1.13E-03	0	1.04E-11
DIMET-01	0	0	0	0	0	0
IODIDE	0.1165571	1.07E-04	0	3.64E-05	0	3.31E-20
HYDRO-01	0	0	0	1.21E-06	0	2.74E-70
ETHAN-01	0	0	0	1.68E-04	0	0.9709922
PROPI-01	0	0	0	0	0	0
LITHI-01	0.0774146	0	0	0.9896943	0	0
Total Flow kmol/hr	1940.368	404.3315	0.5	10404.35	810.9695	338.2567
Total Flow kg/hr	91332.46	26962.1	30.02628	1.35E+06	22715.58	15060.86
Total Flow l/min	1694.432	745.7858	0.4665986	6830.104	33338.23	410.29
Temperature C	170	200	25	70.20361	25	77.7796
Pressure bar	39.31052	38.96579	1	1	10	1.01325
Vapor Frac	0	0	0	0	1	0
Liquid Frac	1	1	1	1	0	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-73583.43	-91696.83	-1.15E+05	-68505.3	-26418.64	-64699.14
Enthalpy cal/gm	-1563.288	-1375.112	-1921.717	-527.0594	-943.1727	-1453.099
Enthalpy cal/sec	-3.97E+07	-1.03E+07	-16028.34	-1.98E+08	-5.95E+06	-6.08E+06
Entropy cal/mol-K	-44.53114	-68.83825	-76.0576	-4.620295	16.72483	-75.12513
Entropy cal/gm-K	-0.946069	-1.032318	-1.266517	-0.0355471	0.5970934	-1.68726
Density mol/cc	0.0190857	9.04E-03	0.0178597	0.0253884	4.05E-04	0.0137405
Density gm/cc	0.8983584	0.6025435	1.072524	3.299902	0.0113561	0.6117972
Average MW	47.06965	66.68315	60.05256	129.9764	28.0104	44.52493
Liq Vol 60F l/min	1426.406	488.5767	0.48025	6645.628	723.8957	315.6682

Table D- 12: Streams Data for Ethanol Standalone Plant Part 5

Stream	H2O	INTR-100	LII	MEI	MEOAC	MEOH
Destination	MAKEUP	R100V	MAKEUP	MAKEUP	MAKEUP	RECYCLE
Source		R-100				T-301
	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	VAPOR
Substream: MIXED						
Mass Frac						
ACETI-01	0	0.3802028	0	0	0	0
WATER	1	0.1003478	0	0	0	9.97E-09
CO2	0	0	0	0	0	0
CO	0	0.1055982	0	0	0	0
METHA-01	0	0.0283345	0	0	0	0.8913564
ACETATE	0	0.2301794	0	0	1	0.0911149
DIMET-01	0	0	0	0	0	0
IODIDE	0	0.0933417	0	1	0	2.19E-04
HYDRO-01	0	0	0	0	0	1.24E-04
ETHAN-01	0	0	0	0	0	0.0171859
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0.0619955	1	0	0	0
Total Flow kmol/hr	0.5	2370.325	10000	55	0.5	389.192
Total Flow kg/hr	9.00764	1.14E+05	1.34E+06	7806.661	37.03972	13200.02
Total Flow l/min	0.1510401	9067.241	6453.283	64.14906	0.6628394	1.76E+05
Temperature C	25	170	25	25	25	63.77682
Pressure bar	1	40	1	1	1	1.01325
Vapor Frac	0	0.2059609	0	0	0	1
Liquid Frac	1	0.7940391	1	1	1	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-68275.29	-74127.78	-69517.38	-3284.076	-1.06E+05	-49692.41
Enthalpy cal/gm	-3789.855	-1540.64	-519.3854	-23.13719	-1433.185	-1465.14
Enthalpy cal/sec	-9482.68	-4.88E+07	-1.93E+08	-50173.39	-14745.77	-5.37E+06
Entropy cal/mol-K	-39.00527	-35.49961	-5.821607	-22.64955	-93.83545	-30.97925
Entropy cal/gm-K	-2.165122	-0.7378086	-0.0434949	-0.1595721	-1.266687	-0.9133981
Density mol/cc	0.055173	4.36E-03	0.0258266	0.0142896	0.0125721	3.68E-05
Density gm/cc	0.993957	0.2096339	3.45678	2.028261	0.9313397	1.25E-03
Average MW	18.01528	48.11493	133.8455	141.9393	74.07944	33.91648
Liq Vol 60F l/min	0.1504167	1919.664	6359.5	57.48417	0.6651925	273.9672

Table D- 13: Streams Data for Ethanol Standalone Plant Part 6

Stream	MEOH-100	MEOH-200	S-100	S-102	S-104	S-105
Destination	P-100	P-201	H-114	I104	E-104	R-100
Source			P-100	C-100	C-101	E-104
	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR	VAPOR
Substream: MIXED						
Mass Frac						
ACETI-01	0	0	0	0	0	0
WATER	0	0	0	0	0	0
CO2	0	0	0	0	0	0
CO	0	0	0	1	1	1
METHA-01	1	1	1	0	0	0
ACETATE	0	0	0	0	0	0
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0	0	0	0
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	675.772	147.1369	675.772	810.9695	810.9695	810.9695
Total Flow kg/hr	21653.19	4714.583	21653.19	22715.58	22715.58	22715.58
Total Flow l/min	455.1357	99.0974	456.6634	19050.24	12537.97	12631.79
Temperature C	25	25	27.22624	148.6753	169.0086	170
Pressure bar	1.01325	1.01325	40	25	40	39.79316
Vapor Frac	0	0	0	1	1	1
Liquid Frac	1	1	1	0	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-57034.64	-57034.64	-56967.32	-25557.99	-25424.03	-25416.69
Enthalpy cal/gm	-1779.988	-1779.988	-1777.886	-912.4463	-907.6638	-907.4017
Enthalpy cal/sec	-1.07E+07	-2.33E+06	-1.07E+07	-5.76E+06	-5.73E+06	-5.73E+06
Entropy cal/mol-K	-57.66153	-57.66153	-57.56606	17.32019	16.69068	16.71765
Entropy cal/gm-K	-1.799552	-1.799552	-1.796572	0.6183485	0.5958743	0.5968374
Density mol/cc	0.0247461	0.0247461	0.0246633	7.10E-04	1.08E-03	1.07E-03
Density gm/cc	0.7929208	0.7929208	0.7902682	0.0198734	0.0301957	0.0299714
Average MW	32.04216	32.04216	32.04216	28.0104	28.0104	28.0104
Liq Vol 60F l/min	454.2832	98.91179	454.2832	723.8957	723.8957	723.8957

Table D- 14: Streams Data for Ethanol Standalone Plant Part 7

Stream	S-106	S-107	S-108	S-109	S-110	S-111
Destination	E-105	VL-100	V-100	B4	RECYCLE	E-107
Source	R100V	E-105	VL-100	V-100	MIX100	RECYCLE
	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	LIQUID
Substream: MIXED						
Mass Frac						
ACETI-01	0.4250917	0.4250917	0.4250917	0.5599429	0.0248477	0.3812415
WATER	0.1121954	0.1121954	0.1121954	0.1157457	5.14E-03	0.0782071
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.0316798	0.0316798	0.0316798	0.0243072	1.08E-03	0.2528221
ACETATE	0.2573557	0.2573557	0.2573557	0.1417513	6.31E-03	0.0937576
DIMET-01	0	0	0	0	0	0
IODIDE	0.1043622	0.1043622	0.1043622	0.0461893	7.59E-03	0.1165571
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0.069315	0.069315	0.069315	0.1120635	0.9550359	0.0774146
Total Flow kmol/hr	1940.368	1940.368	1940.368	1235.612	11279.76	1940.368
Total Flow kg/hr	1.02E+05	1.02E+05	1.02E+05	63093.39	1.41E+06	91332.46
Total Flow l/min	1814.682	1844.922	2.26E+05	987.2025	7493.536	1474.69
Temperature C	170	180	102.1196	102.0998	40.39278	70.20361
Pressure bar	40	39.65526	1.5	1.499	1	1
Vapor Frac	0	0	0.3631366	0	0	0
Liquid Frac	1	1	0.6368634	1	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-85141.98	-84774.01	-84774.01	-90813.19	-71507.5	-76840.45
Enthalpy cal/gm	-1619.599	-1612.599	-1612.599	-1778.473	-572.5349	-1632.484
Enthalpy cal/sec	-4.59E+07	-4.57E+07	-4.57E+07	-3.12E+07	-2.24E+08	-4.14E+07
Entropy cal/mol-K	-47.76949	-46.96572	-45.99663	-52.44869	-9.860931	-52.62236
Entropy cal/gm-K	-0.908687	-0.8933974	-0.874963	-1.027148	-0.0789529	-1.117968
Density mol/cc	0.017821	0.0175289	1.43E-04	0.0208605	0.0250877	0.0219296
Density gm/cc	0.9368472	0.9214911	7.53E-03	1.065188	3.133367	1.032222
Average MW	52.5698	52.5698	52.5698	51.06246	124.8963	47.06965
Liq Vol 60F l/min	1535.871	1535.871	1535.871	934.8518	7343.783	1426.406

Table D- 15: Streams Data for Ethanol Standalone Plant Part 8

Stream	S-112	S-113	S-116	S-117	S-200	S-201
Destination	MIX100	I116	T-100	M-300	P-200	I109
Source	MAKEUP	P-102	V-100	T-100	T-100	P-200
	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED						
Mass Frac						
ACETI-01	2.23E-05	0.3812415	0.2064355	1.18E-20	0.6614495	0.6614495
WATER	6.69E-06	0.0782071	0.1064386	5.28E-03	0.3294157	0.3294157
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0	0.2528221	0.0436343	0.0594138	8.85E-03	8.85E-03
ACETATE	2.75E-05	0.0937576	0.444804	0.6466044	6.35E-06	6.35E-06
DIMET-01	0	0	0	0	0	0
IODIDE	5.80E-03	0.1165571	0.1986875	0.2887057	2.74E-04	2.74E-04
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0.9941451	0.0774146	2.56E-21	0	0	0
Total Flow kmol/hr	10056.5	1940.368	704.7561	345.5563	359.1998	359.1998
Total Flow kg/hr	1.35E+06	91332.46	38911.38	26767.31	12144.07	12144.07
Total Flow l/min	6518.62	1478.285	2.25E+05	428.7856	228.514	228.5555
Temperature C	25.00003	72.238	102.0998	58.52922	112.0486	112.1729
Pressure bar	1	40	1.499	1.41855	1.41855	3.546375
Vapor Frac	0	0	1	0	0	0
Liquid Frac	1	1	0	1	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-69159.19	-76754.51	-74185.83	-80921.48	-83664.22	-83660.06
Enthalpy cal/gm	-516.5862	-1630.658	-1343.641	-1044.667	-2474.638	-2474.515
Enthalpy cal/sec	-1.93E+08	-4.14E+07	-1.45E+07	-7.77E+06	-8.35E+06	-8.35E+06
Entropy cal/mol-K	-5.852529	-52.49831	-34.68333	-71.26301	-45.92236	-45.91637
Entropy cal/gm-K	-0.0437156	-1.115332	-0.6281784	-0.91998	-1.358301	-1.358124
Density mol/cc	0.0257122	0.0218763	5.22E-05	0.0134315	0.0261982	0.0261934
Density gm/cc	3.442287	1.029712	2.88E-03	1.040431	0.8857277	0.8855668
Average MW	133.8773	47.06965	55.21254	77.46148	33.80868	33.80868
Liq Vol 60F l/min	6418.28	1426.406	601.0196	403.4578	197.5618	197.5618

Table D- 16: Streams Data for Ethanol Standalone Plant Part 9

Stream	S-203	S-205	S-206	S-207	S-301	S-302
Destination	I112	T-200	M-300			P-300
Source	P-201	R-200	T-200	T-200	T-300	T-300
	LIQUID	VAPOR	LIQUID	LIQUID	VAPOR	LIQUID
Substream: MIXED						
Mass Frac						
ACETI-01	0	0.0238236	3.92E-23	0.0598806	0	0
WATER	0	0.3730845	0.0152207	0.91471	1.20E-06	0.0109682
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	1	0.0445123	0.057135	0.0254078	0.0593866	0.0585659
ACETATE	0	0.558382	0.927316	1.61E-06	0.1644133	0.9303584
DIMET-01	0	0	0	0	0	0
IODIDE	0	1.98E-04	3.28E-04	1.76E-08	0.7761988	1.07E-04
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	147.1369	506.3367	153.7752	352.5615	95	404.3315
Total Flow kg/hr	4714.583	16858.65	10151.4	6707.252	9956.606	26962.1
Total Flow l/min	99.14054	76817.87	226.8282	159.1174	40140.24	602.8077
Temperature C	25.29005	130	55.2425	97.56714	43.21833	55.12557
Pressure bar	3.546375	3.546375	1.01325	1.01325	1.01325	1.01325
Vapor Frac	0	1	0	0	1	0
Liquid Frac	1	0	1	1	0	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-57027.46	-66996.1	-97157.13	-67638.87	-30045.11	-97546.59
Enthalpy cal/gm	-1779.763	-2012.176	-1471.753	-3555.385	-286.6725	-1462.837
Enthalpy cal/sec	-2.33E+06	-9.42E+06	-4.15E+06	-6.62E+06	-7.93E+05	-1.10E+07
Entropy cal/mol-K	-57.64607	-24.58556	-82.28566	-35.65972	-20.52621	-83.02843
Entropy cal/gm-K	-1.799069	-0.7384083	-1.246477	-1.874426	-0.1958488	-1.245118
Density mol/cc	0.0247354	1.10E-04	0.0112989	0.0369288	3.94E-05	0.0111791
Density gm/cc	0.7925758	3.66E-03	0.7458949	0.7025475	4.13E-03	0.7454589
Average MW	32.04216	33.29534	66.01456	19.02435	104.8064	66.68315
Liq Vol 60F l/min	98.91179	296.2798	183.8302	112.4496	98.71132	488.5767

Table D- 17: Streams Data for Ethanol Standalone Plant Part 10

Stream	S1	S2	S3	S4	H2	S6
Destination	I113	R-300	MIX100		B11	I104
Source	P-300	E-300	B4	B4		C-300
	LIQUID	VAPOR	MIXED	MIXED	VAPOR	VAPOR
Substream: MIXED						
Mass Frac						
ACETI-01	0	0	0.5599429	0.5599429	0	0
WATER	0.0109682	7.63E-05	0.1157457	0.1157457	0	7.63E-05
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.0585659	0.0118304	0.0243072	0.0243072	0	0.0118304
ACETATE	0.9303584	7.62E-03	0.1417513	0.1417513	0	7.62E-03
DIMET-01	0	0	0	0	0	0
IODIDE	1.07E-04	6.81E-05	0.0461893	0.0461893	0	6.81E-05
HYDRO-01	0	0.9742883	0	0	1	0.9742883
ETHAN-01	0	6.12E-03	0	0	0	6.12E-03
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0.1120635	0.1120635	0	0
Total Flow kmol/hr	404.3315	3387.3	1223.256	12.35612	700	3387.3
Total Flow kg/hr	26962.1	6999.765	62462.46	630.9339	1411.116	6999.765
Total Flow l/min	600.7232	56656.1	977.3338	9.872059	21083.58	65942.88
Temperature C	58.0892	200	102.0998	102.0998	50	73.15061
Pressure bar	40	39.89658	1.499	1.499	15	25
Vapor Frac	0	1	8.57E-09	8.57E-09	1	1
Liquid Frac	1	0	1	1	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-97406.17	1160.137	-90813.19	-90813.19	175.863	266.0995
Enthalpy cal/gm	-1460.731	561.4092	-1778.473	-1778.473	87.23882	128.7699
Enthalpy cal/sec	-1.09E+07	1.09E+06	-3.09E+07	-3.12E+05	34195.58	2.50E+05
Entropy cal/mol-K	-82.85477	-4.115766	-52.44869	-52.44869	-4.803359	-5.371826
Entropy cal/gm-K	-1.242514	-1.991686	-1.027148	-1.027148	-2.38276	-2.599514
Density mol/cc	0.0112179	9.96E-04	0.0208604	0.0208604	5.53E-04	8.56E-04
Density gm/cc	0.7480456	2.06E-03	1.065185	1.065185	1.12E-03	1.77E-03
Average MW	66.68315	2.066473	51.06246	51.06246	2.01588	2.066473
Liq Vol 60F l/min	488.5767	3023.406	925.5033	9.348518	624.841	3023.406

Table D- 18: Streams Data for Ethanol Standalone Plant Part 11

Stream	S8	S9	S10	S12	S13	S14
Destination	E-300	P-102	I103	B11	T-301	B12
Source	C-301	E-107	R-300	V-300	V-300	B11
	VAPOR	LIQUID	VAPOR	VAPOR	LIQUID	VAPOR
Substream: MIXED						
Mass Frac						
ACETI-01	0	0.3812415	0	0	0	0
WATER	7.63E-05	0.0782071	8.72E-03	9.51E-05	0.0104642	7.63E-05
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.0118304	0.2528221	0.3530798	0.0147586	0.4213273	0.0118304
ACETATE	7.62E-03	0.0937576	0.0370087	9.51E-03	0.0425577	7.62E-03
DIMET-01	0	0	0	0	0	0
IODIDE	6.81E-05	0.1165571	9.94E-05	8.50E-05	1.02E-04	6.81E-05
HYDRO-01	0.9742883	0	0.1625375	0.9679244	5.78E-05	0.9742883
ETHAN-01	6.12E-03	0	0.4385512	7.63E-03	0.5254907	6.12E-03
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0.0774146	0	0	0	0
Total Flow kmol/hr	3387.3	1940.368	3469.263	2741.808	727.4487	3441.808
Total Flow kg/hr	6999.765	91332.46	33961.87	5701.287	28260.88	7112.403
Total Flow l/min	51204.62	1996.836	57288.85	42229.9	725.5971	91080.45
Temperature C	154.9037	52.08151	200	0.2575611	0.2575611	10.58781
Pressure bar	40	0.6552621	40	24.999	24.999	15
Vapor Frac	1	0	1	1	0	1
Liquid Frac	0	1	0	0	1	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	843.2274	-76816.7	-9673.443	-258.1093	-63153.51	-169.8473
Enthalpy cal/gm	408.0514	-1631.979	-988.1589	-124.1274	-1625.602	-82.19188
Enthalpy cal/sec	7.93E+05	-4.14E+07	-9.32E+06	-1.97E+05	-1.28E+07	-1.62E+05
Entropy cal/mol-K	-4.824889	-54.11949	-10.7375	-7.019033	-70.24872	-5.733539
Entropy cal/gm-K	-2.334842	-1.149775	-1.096854	-3.375525	-1.808236	-2.774553
Density mol/cc	1.10E-03	0.0161953	1.01E-03	1.08E-03	0.0167092	6.30E-04
Density gm/cc	2.28E-03	0.7623098	9.88E-03	2.25E-03	0.6491408	1.30E-03
Average MW	2.066473	47.06965	9.78936	2.07939	38.84931	2.066473
Liq Vol 60F l/min	3023.406	1426.406	3036.858	2447.217	589.6354	3072.058

Table D- 19: Streams Data for Ethanol Standalone Plant Part 12

Stream	S15	S16	S17	S18	S22	VENT
Destination		C-300	V-300	R-200	T-300	
Source	B12	B12	VL-300	B17	M-300	R100V
	VAPOR	VAPOR	MIXED	MIXED	MIXED	VAPOR
Substream: MIXED						
Mass Frac						
ACETI-01	0	0	0	0.4764727	8.58E-21	0
WATER	7.63E-05	7.63E-05	8.72E-03	0.2372934	8.01E-03	0
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	1
METHA-01	0.0118304	0.0118304	0.3530759	0.2860317	0.0587872	0
ACETATE	7.62E-03	7.62E-03	0.0370092	4.58E-06	0.7237906	0
DIMET-01	0	0	0	0	0	0
IODIDE	6.81E-05	6.81E-05	9.94E-05	1.98E-04	0.2094116	0
HYDRO-01	0.9742883	0.9742883	0.1625353	0	0	0
ETHAN-01	6.12E-03	6.12E-03	0.4385567	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	54.50761	3387.3	3469.256	506.3367	499.3315	429.9569
Total Flow kg/hr	112.6385	6999.765	33962.17	16858.65	36918.71	12043.27
Total Flow l/min	1442.433	89638.01	42953.82	19633.93	6729.154	6662.769
Temperature C	10.58781	10.58781	0.2575262	124.3077	50.74544	170
Pressure bar	15	15	25	3.201637	1.01325	40
Vapor Frac	1	1	0.7903156	0.2293729	0.0288396	1
Liquid Frac	0	0	0.2096844	0.7706271	0.9711603	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-169.8473	-169.8473	-13446.29	-72688.13	-85921.44	-25416.85
Enthalpy cal/gm	-82.19188	-82.19188	-1373.547	-2183.132	-1162.101	-907.4075
Enthalpy cal/sec	-2571.659	-1.60E+05	-1.30E+07	-1.02E+07	-1.19E+07	-3.04E+06
Entropy cal/mol-K	-5.733539	-5.733539	-20.27737	-40.1552	-74.54903	16.7069
Entropy cal/gm-K	-2.774553	-2.774553	-2.071346	-1.206031	-1.008288	0.5964534
Density mol/cc	6.30E-04	6.30E-04	1.35E-03	4.30E-04	1.24E-03	1.08E-03
Density gm/cc	1.30E-03	1.30E-03	0.0131777	0.0143108	0.0914396	0.0301257
Average MW	2.066473	2.066473	9.789466	33.29534	73.93626	28.0104
Liq Vol 60F l/min	48.65191	3023.406	3036.852	296.4736	587.288	383.7924

APPENDIX D.3 STREAMS DATA OF STRUCTURALLY INTEGRATED PLANT

Table D- 20:Streams Data for Structurally Integrated Plant part 1

Stream	3-S10	36-S203	59-S10	89-S115	90-S115	94-S203
Destination	VL-300	I121	C132	T-100	I125	H119
Source	C132	I125	C129	I125	I122	I121
	MIXED	LIQUID	MIXED	MIXED	MIXED	MIXED
Mass Frac						
ACETI-01	0	0	0	0.6797606	0.6797606	0
WATER	9.42E-03	0	9.42E-03	0.027006	0.027006	0
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.3555276	1	0.3555276	0	0	1
ACETATE	0.0368294	0	0.0368294	0.0445131	0.0445131	0
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0	0.2487203	0.2487203	0
HYDRO-01	0.1618081	0	0.1618081	0	0	0
ETHAN-01	0.4364147	0	0.4364147	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	6.60E-19	6.60E-19	0
Total Flow kmol/hr	3474.906	392.1926	3474.906	1341.899	1341.899	392.1926
Total Flow kg/hr	34116.05	12566.7	34116.05	88447.63	88447.63	12566.7
Total Flow l/min	30183.96	284.1893	36812.02	15162.65	28494.5	5881.944
Temperature C	3	69.94056	59.76	89.10939	92.49936	96.46341
Pressure bar	36.58631	3.201637	36.61217	1.312842	1.333526	3.149926
Vapor Frac	0.7881492	0	0.804137	0.0307896	0.0616345	0.0949283
Liquid Frac	0.2118508	1	0.195863	0.9692103	0.9383655	0.9050716
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-13520.27	-56070.43	-12736.97	-95234.7	-94954.36	-54667.5
Enthalpy cal/gm	-1377.114	-1749.896	-1297.33	-1444.87	-1440.617	-1706.111
Enthalpy cal/sec	-1.31E+07	-6.11E+06	-1.23E+07	-3.55E+07	-3.54E+07	-5.96E+06
Entropy cal/mol-K	-20.91952	-54.70451	-18.3549	-59.04644	-58.27951	-50.86739
Entropy cal/gm-K	-2.130767	-1.707266	-1.869547	-0.8958333	-0.8841977	-1.587514
Density mol/cc	1.92E-03	0.0230006	1.57E-03	1.48E-03	7.85E-04	1.11E-03
Density gm/cc	0.0188378	0.7369911	0.015446	0.0972209	0.0517337	0.0356081
Average MW	9.817833	32.04216	9.817833	65.91231	65.91231	32.04216
Liq Vol 60F l/min	3040.106	263.6489	3040.106	1234.21	1234.21	263.6489

Table D- 21: Streams Data for Structurally Integrated Plant part 2

Stream	95-115	98-S10	100-S203	102-S10	108-S203	110-S115
Destination	I122	C129	I112	I121	H109	C120
Source	C120	I121	H119	I118	I112	I112
	MIXED	MIXED	VAPOR	MIXED	VAPOR	MIXED
Mass Frac						
ACETI-01	0.6797606	0	0	0	0	0.6797606
WATER	0.027006	9.42E-03	0	9.42E-03	0	0.027006
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0	0.3555276	1	0.3555276	1	0
ACETATE	0.0445131	0.0368294	0	0.0368294	0	0.0445131
DIMET-01	0	0	0	0	0	0
IODIDE	0.2487203	0	0	0	0	0.2487203
HYDRO-01	0	0.1618081	0	0.1618081	0	0
ETHAN-01	0	0.4364147	0	0.4364147	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	6.60E-19	0	0	0	0	6.60E-19
Total Flow kmol/hr	1341.899	3474.906	392.1926	3474.906	392.1926	1341.899
Total Flow kg/hr	88447.63	34116.05	12566.7	34116.05	12566.7	88447.63
Total Flow l/min	40572.78	43409.32	61074.7	44471.6	68119.26	3.35E+05
Temperature C	95.55	98.43	100.2	103.1145	109.86	117.4302
Pressure bar	1.35421	36.63803	3.098216	36.66388	2.891373	1.374894
Vapor Frac	0.0907554	0.8616975	1	0.8749826	1	0.8625369
Liquid Frac	0.9092446	0.1383025	0	0.1250174	0	0.1374631
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-94694.02	-11814.47	-47467.44	-11656.13	-47287.1	-89520.06
Enthalpy cal/gm	-1436.667	-1203.368	-1481.406	-1187.24	-1475.778	-1358.169
Enthalpy cal/sec	-3.53E+07	-1.14E+07	-5.17E+06	-1.13E+07	-5.15E+06	-3.34E+07
Entropy cal/mol-K	-57.57439	-15.74691	-31.35783	-15.32468	-30.7519	-44.09039
Entropy cal/gm-K	-0.8734999	-1.603909	-0.9786429	-1.560903	-0.9597326	-0.668925
Density mol/cc	5.51E-04	1.33E-03	1.07E-04	1.30E-03	9.60E-05	6.67E-05
Density gm/cc	0.0363329	0.0130985	3.43E-03	0.0127857	3.07E-03	4.40E-03
Average MW	65.91231	9.817833	32.04216	9.817833	32.04216	65.91231
Liq Vol 60F l/min	1234.21	3040.106	263.6489	3040.106	263.6489	1234.21

Table D- 22: Streams Data for Structurally Integrated Plant part 3

Stream	114-S100	117-S10	117-S115	130-S203	131-S115	141-S109
Destination	H117	I118	I112	B17	C111	H110
Source	I118	I116	C111	H109	V-100	I116
	LIQUID	MIXED	MIXED	VAPOR	VAPOR	LIQUID
Mass Frac						
ACETI-01	0	0	0.6797606	0	0.6797606	0.4374472
WATER	0	9.42E-03	0.027006	0	0.027006	0.0342315
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	1	0.3555276	0	1	0	0
ACETATE	0	0.0368294	0.0445131	0	0.0445131	0.0496483
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0.2487203	0	0.2487203	0.2602262
HYDRO-01	0	0.1618081	0	0	0	0
ETHAN-01	0	0.4364147	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	6.60E-19	0	6.60E-19	0.2184468
Total Flow kmol/hr	999.9326	3474.906	1341.899	392.1926	1341.899	1237.66
Total Flow kg/hr	32040	34116.05	88447.63	12566.7	88447.63	92916.06
Total Flow l/min	790.7291	48504.44	3.33E+05	78595.73	3.77E+05	1136.39
Temperature C	114.29	117.54	117.99	130	131.3168	132.2143
Pressure bar	29.65526	36.68974	1.395579	2.68453	1.499	29.65526
Vapor Frac	0	0.9313289	0.8688717	1	1	0
Liquid Frac	1	0.068671	0.1311283	0	0	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-54928.47	-11063.34	-89467.35	-46961.66	-88123.78	-83726
Enthalpy cal/gm	-1714.256	-1126.862	-1357.37	-1465.621	-1336.985	-1115.246
Enthalpy cal/sec	-1.53E+07	-1.07E+07	-3.33E+07	-5.12E+06	-3.28E+07	-2.88E+07
Entropy cal/mol-K	-51.70356	-13.78146	-43.97455	-29.78265	-40.67305	-43.6675
Entropy cal/gm-K	-1.61361	-1.403717	-0.6671676	-0.9294833	-0.6170782	-0.5816595
Density mol/cc	0.0210761	1.19E-03	6.71E-05	8.32E-05	5.93E-05	0.0181519
Density gm/cc	0.6753261	0.0117226	4.42E-03	2.66E-03	3.91E-03	1.362737
Average MW	32.04216	9.817833	65.91231	32.04216	65.91231	75.074
Liq Vol 60F l/min	672.198	3040.106	1234.21	263.6489	1234.21	1060.545

Table D- 23: Streams Data for Structurally Integrated Plant part 4

Stream	149-S10	157-S100	177-S10	180-S100	180-S109	ACOH
Destination	I116	I107	C115	B1	R-100	MAKEUPX
Source	C115	H117	I107	I107	H110	
	VAPOR	LIQUID	VAPOR	LIQUID	LIQUID	LIQUID
Mass Frac						
ACETI-01	0	0	0	0	0.4374472	1
WATER	9.42E-03	0	9.42E-03	0	0.0342315	0
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.3555276	1	0.3555276	1	0	0
ACETATE	0.0368294	0	0.0368294	0	0.0496483	0
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0	0	0.2602262	0
HYDRO-01	0.1618081	0	0.1618081	0	0	0
ETHAN-01	0.4364147	0	0.4364147	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0.2184468	0
Total Flow kmol/hr	3474.906	999.9326	3474.906	999.9326	1237.66	500
Total Flow kg/hr	34116.05	32040	34116.05	32040	92916.06	30026.28
Total Flow l/min	55563.75	881.4339	55018.96	951.4247	1191.08	466.5986
Temperature C	149.06	157.02	176.6558	180	180	25
Pressure bar	36.79316	29.31052	39.79316	28.96579	29.31052	1.01325
Vapor Frac	1	0	1	0	0	0
Liquid Frac	0	1	0	1	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-10234.67	-53649	-9966.743	-52846.51	-81879.43	-1.15E+05
Enthalpy cal/gm	-1042.457	-1674.325	-1015.167	-1649.28	-1090.65	-1921.717
Enthalpy cal/sec	-9.88E+06	-1.49E+07	-9.62E+06	-1.47E+07	-2.82E+07	-1.60E+07
Entropy cal/mol-K	-11.71711	-48.65981	-11.25933	-46.90876	-39.41638	-76.05761
Entropy cal/gm-K	-1.193451	-1.518618	-1.146825	-1.46397	-0.5250336	-1.266517
Density mol/cc	1.04E-03	0.0189073	1.05E-03	0.0175164	0.0173184	0.0178597
Density gm/cc	0.0102333	0.605831	0.0103346	0.5612636	1.300165	1.072524
Average MW	9.817833	32.04216	9.817833	32.04216	75.074	60.05256
Liq Vol 60F l/min	3040.106	672.198	3040.106	672.198	1060.545	480.25

Table D- 24: Streams Data for Structurally Integrated Plant part 5

Stream	ACOH-E	ACOH-P	BLEEDX	COX	ETOH	H2O
Destination	P-200			CX-100		MAKEUPX
Source	B9	B9	RECYCLEX		T-300	
	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID	LIQUID
Mass Frac						
ACETI-01	0.9984403	0.9984403	0.159775	0	0	0
WATER	1.56E-03	1.56E-03	0.0357508	0	0.0213333	1
CO2	0	0	0	0	0	0
CO	0	0	0	1	0	0
METHA-01	0	0	0	0	7.07E-03	0
ACETATE	1.20E-12	1.20E-12	0.1789724	0	8.45E-12	0
DIMET-01	0	0	0	0	0	0
IODIDE	1.12E-23	1.12E-23	0.2647018	0	0	0
HYDRO-01	0	0	0	0	3.05E-70	0
ETHAN-01	0	0	0	0	0.9715929	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0.3608	0	0	0
Total Flow kmol/hr	358.1816	638	2149.077	1159.333	338.257	500
Total Flow kg/hr	21431.72	38174.6	1.85E+05	32473.39	15037.07	9007.64
Total Flow l/min	377.9595	673.2287	1838.57	47659.16	409.4614	151.0401
Temperature C	117.7511	117.7511	53.98696	25	77.84492	25
Pressure bar	1.01325	1.01325	1.01325	10	1.01325	1.01325
Vapor Frac	0	0	0	1	0	0
Liquid Frac	1	1	1	0	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-1.12E+05	-1.12E+05	-76022.88	-26418.64	-64735.16	-68275.29
Enthalpy cal/gm	-1878.302	-1878.302	-883.5037	-943.1727	-1456.209	-3789.854
Enthalpy cal/sec	-1.12E+07	-1.99E+07	-4.54E+07	-8.51E+06	-6.08E+06	-9.48E+06
Entropy cal/mol-K	-67.735	-67.735	-43.08667	16.72483	-75.03101	-39.00528
Entropy cal/gm-K	-1.132034	-1.132034	-0.5007339	0.5970934	-1.687813	-2.165122
Density mol/cc	0.0157945	0.0157945	0.0194814	4.05E-04	0.0137683	0.055173
Density gm/cc	0.9450625	0.9450625	1.676319	0.0113561	0.6120671	0.993957
Average MW	59.83479	59.83479	86.04705	28.0104	44.45457	18.01528
Liq Vol 60F l/min	342.8094	610.6187	1854.775	1034.856	315.061	150.4167

Table D- 25: Streams Data for Structurally Integrated Plant part 6

Stream	INTR-100	LII	MEI	MEOAC	MEOH	MEOH-200
Destination	RVX	MAKEUPX	MAKEUPX	MAKEUPX		P-201
Source	R-100				T-300	
	MIXED	LIQUID	LIQUID	LIQUID	VAPOR	LIQUID
Mass Frac						
ACETI-01	0.6396159	0	0	0	0	0
WATER	0.0202036	0	0	0	1.16E-08	0
CO2	0	0	0	0	0	0
CO	0.0283611	0	0	0	0	0
METHA-01	0	0	0	0	0.8923997	1
ACETATE	0.0293028	0	0	1	0.0898822	0
DIMET-01	0	0	0	0	0	0
IODIDE	0.1535875	0	1	0	0	0
HYDRO-01	0	0	0	0	1.22E-04	0
ETHAN-01	0	0	0	0	0.0175957	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0.128929	1	0	0	0	0
Total Flow kmol/hr	2396.993	500	500	500	394.7233	392.1926
Total Flow kg/hr	1.57E+05	66922.74	70969.65	37039.72	13377.4	12566.7
Total Flow l/min	5087.03	322.6641	583.1733	662.8394	1.79E+05	264.1436
Temperature C	180	25	25	25	63.7924	25
Pressure bar	30	1.01325	1.01325	1.01325	1.01325	1.01325
Vapor Frac	0.0566661	0	0	0	1	0
Liquid Frac	0.9433338	1	1	1	0	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-89894.53	-69517.37	-3284.064	-1.06E+05	-49668.7	-57034.64
Enthalpy cal/gm	-1368.718	-519.3853	-23.1371	-1433.185	-1465.561	-1779.988
Enthalpy cal/sec	-5.99E+07	-9.66E+06	-4.56E+05	-1.47E+07	-5.45E+06	-6.21E+06
Entropy cal/mol-K	-44.79008	-5.82161	-22.64957	-93.83548	-30.96749	-57.66153
Entropy cal/gm-K	-0.6819658	-0.043495	-0.1595723	-1.266687	-0.9137493	-1.799552
Density mol/cc	7.85E-03	0.0258266	0.0142896	0.0125721	3.68E-05	0.0247461
Density gm/cc	0.515787	3.45678	2.028261	0.9313397	1.25E-03	0.7929208
Average MW	65.67789	133.8455	141.9393	74.07944	33.89057	32.04216
Liq Vol 60F l/min	2163.267	317.975	522.5833	665.1925	277.7304	263.6489

Table D- 26: Streams Data for Structurally Integrated Plant part 7

Stream	MEOHX	QS1	S-201	S-202	S-203	S-205
Destination	B2	R-100	E-200	B17	I125	T-200
Source		B1	P-200	E-200	P-201	R-200
	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	VAPOR
Mass Frac						
ACETI-01	0	0	0.9984403	0.9984403	0	0.0314695
WATER	0	0	1.56E-03	1.56E-03	0	0.1803547
CO2	0	0	0	0	0	0
CO	0	0.5033589	0	0	0	0
METHA-01	1	0.4966411	0	0	1	0.0505939
ACETATE	0	0	1.20E-12	1.20E-12	0	0.7375817
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	1.12E-23	1.12E-23	0	0
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	999.9326	2159.266	358.1816	358.1816	392.1926	750.3742
Total Flow kg/hr	32040	64513.39	21431.72	21431.72	12566.7	33998.42
Total Flow l/min	673.4594	27503.6	378.0521	385.4235	264.2142	1.13E+05
Temperature C	25	118.1432	117.9079	130	25.17811	130
Pressure bar	1.01325	28.96579	3.546375	3.201637	3.546375	3.546375
Vapor Frac	0	0.6912941	0	0	0	1
Liquid Frac	1	0.3087059	1	1	1	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-57034.64	-38076.34	-1.12E+05	-1.12E+05	-57029.63	-75063.93
Enthalpy cal/gm	-1779.988	-1274.417	-1878.182	-1871.297	-1779.831	-1656.725
Enthalpy cal/sec	-1.58E+07	-2.28E+07	-1.12E+07	-1.11E+07	-6.21E+06	-1.56E+07
Entropy cal/mol-K	-57.66153	-11.72762	-67.72683	-66.71231	-57.65319	-36.15674
Entropy cal/gm-K	-1.799552	-0.3925241	-1.131897	-1.114942	-1.799292	-0.7980102
Density mol/cc	0.0247461	1.31E-03	0.0157906	0.0154886	0.0247395	1.11E-04
Density gm/cc	0.7929208	0.0390939	0.944831	0.9267606	0.792709	5.01E-03
Average MW	32.04216	29.87746	59.83479	59.83479	32.04216	45.30862
Liq Vol 60F l/min	672.198	1707.054	342.8094	342.8094	263.6489	605.9421

Table D- 27: Streams Data for Structurally Integrated Plant part 8

Stream	S1	S2	S4	H2	S6	S7
Destination	H131	R-300		B11	E-301	C-301
Source	P-300	E-300	B4		C-300	E-301
	LIQUID	VAPOR	LIQUID	VAPOR	VAPOR	VAPOR
Mass Frac						
ACETI-01	5.84E-21	0	0.6288452	0	0	0
WATER	0.0118301	8.24E-05	0.0122764	0	8.24E-05	8.24E-05
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.0634318	0.0119282	0	0	0.0119282	0.0119282
ACETATE	0.924738	7.60E-03	0.0104785	0	7.60E-03	7.60E-03
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0.0337969	0	0	0
HYDRO-01	0	0.974277	0	1	0.974277	0.974277
ETHAN-01	0	6.11E-03	0	0	6.11E-03	6.11E-03
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0.3146029	0	0	0
Total Flow kmol/hr	410	3387.167	8.956935	700	3387.167	3387.167
Total Flow kg/hr	27117.53	6999.535	645.1693	1411.116	6999.535	6999.535
Total Flow l/min	511.3391	57230.26	8.019785	21160.93	65965.43	68053.44
Temperature C	57.60806	200	131.3168	50	73.28394	82.22222
Pressure bar	40	39.79316	1.499	15	25	24.85
Vapor Frac	0	1	0	1	1	1
Liquid Frac	1	0	1	0	0	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-96888.58	1164.291	-1.00E+05	177.4411	266.7471	329.0532
Enthalpy cal/gm	-1464.894	563.4157	-1392.745	88.02166	129.0824	159.2332
Enthalpy cal/sec	-1.10E+07	1.10E+06	-2.50E+05	34502.44	2.51E+05	3.10E+05
Entropy cal/mol-K	-82.37414	-4.116632	-51.36059	-4.805862	-5.369228	-5.179541
Entropy cal/gm-K	-1.245445	-1.992092	-0.713043	-2.384002	-2.59824	-2.506448
Density mol/cc	0.0133636	9.86E-04	0.0186142	5.51E-04	8.56E-04	8.30E-04
Density gm/cc	0.8838731	2.04E-03	1.340787	1.11E-03	1.77E-03	1.71E-03
Average MW	66.14032	2.066486	72.03015	2.01588	2.066486	2.066486
Liq Vol 60F l/min	491.7933	3023.28	7.867709	624.841	3023.28	3023.28

Table D- 28: Streams Data for Structurally Integrated Plant part 9

Stream	S8	S9	S10	S12	S13	S14
Destination	E-300	P-300	I107	B11	T-300	B12
Source	C-301	T-200	R-300	V-300	V-300	B11
	VAPOR	LIQUID	VAPOR	VAPOR	LIQUID	VAPOR
Mass Frac						
ACETI-01	0	5.84E-21	0	0	0	0
WATER	8.24E-05	0.0118301	9.42E-03	1.03E-04	0.0112896	8.24E-05
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.0119282	0.0634318	0.3555276	0.0148804	0.4238811	0.0119282
ACETATE	7.60E-03	0.924738	0.0368294	9.49E-03	0.0423161	7.60E-03
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0	0	0	0
HYDRO-01	0.974277	0	0.1618081	0.9679106	5.76E-05	0.974277
ETHAN-01	6.11E-03	0	0.4364147	7.62E-03	0.5224555	6.11E-03
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	3387.167	410	3474.906	2741.926	732.9803	3441.926
Total Flow kg/hr	6999.535	27117.53	34116.05	5701.577	28414.47	7112.693
Total Flow l/min	51106.76	509.0904	57372.55	42244.1	729.7653	91407.86
Temperature C	154.0898	54.92032	200	0.338466	0.338466	10.45788
Pressure bar	40	1.01325	40	24.999	24.999	15
Vapor Frac	1	0	1	1	0	1
Liquid Frac	0	1	0	0	1	0
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	837.2292	-97009.69	-9735.819	-257.9061	-63132.01	-169.3675
Enthalpy cal/gm	405.1462	-1466.725	-991.6464	-124.0287	-1628.555	-81.95918
Enthalpy cal/sec	7.88E+05	-1.10E+07	-9.40E+06	-1.96E+05	-1.29E+07	-1.62E+05
Entropy cal/mol-K	-4.838341	-82.52966	-10.75596	-7.017109	-70.11017	-5.739061
Entropy cal/gm-K	-2.341337	-1.247796	-1.095553	-3.374574	-1.808564	-2.777207
Density mol/cc	1.10E-03	0.0134226	1.01E-03	1.08E-03	0.01674	6.28E-04
Density gm/cc	2.28E-03	0.8877773	9.91E-03	2.25E-03	0.6489408	1.30E-03
Average MW	2.066486	66.14032	9.817833	2.079406	38.76566	2.066486
Liq Vol 60F l/min	3023.28	491.7933	3040.106	2447.314	592.7914	3072.155

Table D- 29: Streams Data for Structurally Integrated Plant part 10

Stream	S15	S16	S17	S18	S21	S21-200
Destination		C-300	V-300	R-200	H108	R-300
Source	B12	B12	VL-300	B17	H131	H108
	VAPOR	VAPOR	MIXED	MIXED	LIQUID	LIQUID
Mass Frac						
ACETI-01	0	0	0	0.6293908	5.84E-21	5.84E-21
WATER	8.24E-05	8.24E-05	9.42E-03	9.83E-04	0.0118301	0.0118301
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0.0119282	0.0119282	0.3555276	0.369626	0.0634318	0.0634318
ACETATE	7.60E-03	7.60E-03	0.0368294	7.54E-13	0.924738	0.924738
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0	7.09E-24	0	0
HYDRO-01	0.974277	0.974277	0.1618081	0	0	0
ETHAN-01	6.11E-03	6.11E-03	0.4364147	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0	0
Total Flow kmol/hr	54.75854	3387.167	3474.906	750.3742	410	410
Total Flow kg/hr	113.1578	6999.535	34116.05	33998.42	27117.53	27117.53
Total Flow l/min	1454.233	89953.63	42972.2	75588.93	577.511	750.586
Temperature C	10.45788	10.45788	0.3384668	125.0712	120.99	200
Pressure bar	15	15	25	2.68453	39.65526	39.31052
Vapor Frac	1	1	0.7890646	0.5608021	0	0
Liquid Frac	0	0	0.2109354	0.4391979	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-169.3675	-169.3675	-13520.27	-77991.94	-94727.12	-91171.91
Enthalpy cal/gm	-81.95918	-81.95918	-1377.114	-1721.349	-1432.214	-1378.462
Enthalpy cal/sec	-2576.2	-1.59E+05	-1.31E+07	-1.63E+07	-1.08E+07	-1.04E+07
Entropy cal/mol-K	-5.739061	-5.739061	-20.32573	-46.70278	-76.3757	-68.38541
Entropy cal/gm-K	-2.777207	-2.777207	-2.070287	-1.03077	-1.154752	-1.033944
Density mol/cc	6.28E-04	6.28E-04	1.35E-03	1.65E-04	0.0118323	9.10E-03
Density gm/cc	1.30E-03	1.30E-03	0.0132318	7.50E-03	0.7825979	0.6021414
Average MW	2.066486	2.066486	9.817833	45.30862	66.14032	66.14032
Liq Vol 60F l/min	48.87577	3023.28	3040.106	606.4583	491.7933	491.7933

Table D- 30: Streams Data for Structurally Integrated Plant part 11

Stream	S22	SX-100	SX-102	SX-103	SX-104	SX-105
Destination		I118	EX-101	B1	MIX100	MIX100
Source	T-200	B2	CX-100	EX-101	MAKEUPX	B4
	LIQUID	LIQUID	VAPOR	VAPOR	LIQUID	LIQUID
Mass Frac						
ACETI-01	0.1554908	0	0	0	0.140332	0.6288452
WATER	0.8445091	0	0	0	0.0420984	0.0122764
CO2	0	0	0	0	0	0
CO	0	0	1	1	0	0
METHA-01	7.99E-08	1	0	0	0	0
ACETATE	1.50E-19	0	0	0	0.1731103	0.0104785
DIMET-01	0	0	0	0	0	0
IODIDE	0	0	0	0	0.3316865	0.0337969
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0	0	0	0	0.3127727	0.3146029
Total Flow kmol/hr	340.3742	999.9326	1159.333	1159.333	2500	886.7366
Total Flow kg/hr	6880.886	32040	32473.39	32473.39	2.14E+05	63871.77
Total Flow l/min	126.4009	674.9347	24299.17	24619.68	2097.708	793.9587
Temperature C	100.5007	26.45561	177.2494	180	24.89574	131.3168
Pressure bar	1.01325	30	30	29.79316	1.01325	1.499
Vapor Frac	0	0	1	1	0	0
Liquid Frac	1	1	0	0	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-69352.52	-56988.49	-25356.91	-25336.97	-72530.06	-1.00E+05
Enthalpy cal/gm	-3430.635	-1778.547	-905.2678	-904.5557	-847.4484	-1392.745
Enthalpy cal/sec	-6.56E+06	-1.58E+07	-8.17E+06	-8.16E+06	-5.04E+07	-2.47E+07
Entropy cal/mol-K	-36.46645	-57.60321	17.41715	17.47514	-44.68318	-51.36059
Entropy cal/gm-K	-1.803872	-1.797732	0.6218101	0.6238805	-0.5220826	-0.713043
Density mol/cc	0.0448802	0.024692	7.95E-04	7.85E-04	0.0198629	0.0186142
Density gm/cc	0.9072836	0.7911876	0.0222733	0.0219833	1.699998	1.340787
Average MW	20.21565	32.04216	28.0104	28.0104	85.58641	72.03015
Liq Vol 60F l/min	114.1487	672.198	1034.856	1034.856	2136.418	778.9032

Table D- 31: Streams Data for Structurally Integrated Plant part 12

Stream	SX-106	SX-107	SX-108	SX-109	SX-111	SX-112
Destination	RECYCLEX	I122	PX-101	I116	EX-102	VLX-100
Source	MIX100	RECYCLEX	I122	PX-101	RVX	EX-102
	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
Mass Frac						
ACETI-01	0.2526357	0.4374472	0.4374472	0.4374472	0.6582856	0.6582856
WATER	0.0352427	0.0342315	0.0342315	0.0342315	0.0207934	0.0207934
CO2	0	0	0	0	0	0
CO	0	0	0	0	0	0
METHA-01	0	0	0	0	0	0
ACETATE	0.1357231	0.0496483	0.0496483	0.0496483	0.0301581	0.0301581
DIMET-01	0	0	0	0	0	0
IODIDE	0.2632051	0.2602262	0.2602262	0.2602262	0.1580706	0.1580706
HYDRO-01	0	0	0	0	0	0
ETHAN-01	0	0	0	0	0	0
PROPI-01	0	0	0	0	0	0
LITHI-01	0.3131935	0.2184468	0.2184468	0.2184468	0.1326923	0.1326923
Total Flow kmol/hr	3386.737	1237.66	1237.66	1237.66	2237.592	2237.592
Total Flow kg/hr	2.78E+05	92916.06	92916.06	92916.06	1.53E+05	1.53E+05
Total Flow l/min	2894.253	1061.53	1069.337	1070.212	2330.636	2434.364
Temperature C	53.98696	53.98696	62.93033	63.91988	180	210.7
Pressure bar	1.01325	1.01325	0.6685121	30	30	29.65526
Vapor Frac	0	0	0	0	0	0
Liquid Frac	1	1	1	1	1	1
Solid Frac	0	0	0	0	0	0
Enthalpy cal/mol	-79806.09	-86390.15	-86107.88	-86052.63	-94423.5	-93005.68
Enthalpy cal/gm	-972.8058	-1150.733	-1146.973	-1146.237	-1381.243	-1360.503
Enthalpy cal/sec	-7.51E+07	-2.97E+07	-2.96E+07	-2.96E+07	-5.87E+07	-5.78E+07
Entropy cal/mol-K	-45.82234	-50.95291	-50.07468	-50.01926	-49.15289	-46.24949
Entropy cal/gm-K	-0.5585568	-0.6787024	-0.6670043	-0.6662661	-0.719017	-0.6765455
Density mol/cc	0.0195026	0.019432	0.0192901	0.0192743	0.0160013	0.0153194
Density gm/cc	1.59994	1.458839	1.448188	1.447004	1.093869	1.047259
Average MW	82.03702	75.074	75.074	75.074	68.36124	68.36124
Liq Vol 60F l/min	2915.321	1060.545	1060.545	1060.545	2020.981	2020.981

Table D- 32: Streams Data for Structurally Integrated Plant part 13

Stream	SX-113	SX-114	SX-116	SX-117	VENTX
Destination	V-100	B4		B9	
Source	VLX-100	V-100	T-100	T-100	RVX
	MIXED	LIQUID	LIQUID	LIQUID	VAPOR
Mass Frac					
ACETI-01	0.6582856	0.6288452	0.0211456	0.9984403	0
WATER	0.0207934	0.0122764	0.0795958	1.56E-03	0
CO2	0	0	0	0	0
CO	0	0	0	0	1
METHA-01	0	0	0	0	0
ACETATE	0.0301581	0.0104785	0.1365083	1.20E-12	0
DIMET-01	0	0	0	0	0
IODIDE	0.1580706	0.0337969	0.7627502	1.12E-23	0
HYDRO-01	0	0	0	0	0
ETHAN-01	0	0	0	0	0
PROPI-01	0	0	0	0	0
LITHI-01	0.1326923	0.3146029	0	0	0
Total Flow kmol/hr	2237.592	895.6935	345.717	996.1816	159.4007
Total Flow kg/hr	1.53E+05	64516.93	28841.32	59606.32	4464.879
Total Flow l/min	3.78E+05	801.9785	301.1607	1051.188	3361.881
Temperature C	131.3373	131.3168	54.10422	117.7511	180
Pressure bar	1.5	1.499	1.01325	1.01325	30
Vapor Frac	0.599605	0	0	0	1
Liquid Frac	0.400395	1	1	1	0
Solid Frac	0	0	0	0	0
Enthalpy cal/mol	-93005.68	-1.00E+05	-45577.87	-1.12E+05	-25337.12
Enthalpy cal/gm	-1360.503	-1392.745	-546.3359	-1878.302	-904.561
Enthalpy cal/sec	-5.78E+07	-2.50E+07	-4.38E+06	-3.11E+07	-1.12E+06
Entropy cal/mol-K	-44.9518	-51.36059	-36.91192	-67.735	17.46097
Entropy cal/gm-K	-0.6575627	-0.713043	-0.4424583	-1.132034	0.6233744
Density mol/cc	9.87E-05	0.0186142	0.0191324	0.0157945	7.90E-04
Density gm/cc	6.75E-03	1.340787	1.59612	0.9450625	0.0221348
Average MW	68.36124	72.03015	83.42464	59.83479	28.0104
Liq Vol 60F l/min	2020.981	786.7709	280.7817	953.4281	142.2859

APPENDIX E

ECONOMICS SUMMARY OF SIMULATED PLANTS

APPENDIX E.1 ECONOMICS SUMMARY OF ACETIC ACID STANDALONE PLANT

Table E- 1: Investment Summary for Acetic Acid Standalone Plant

INVESTMENT	Value	Units
Currency Conversion Rate	1	USD/U.S. DOLLAR
Total Project Capital Cost	1.49E+07	USD
Total Operating Cost	8.44E+06	USD/Year
Total Raw Materials Cost	0	USD/Year
Total Utilities Cost	5.81E+06	USD/Year
Total Product Sales	0	USD/Year
Desired Rate of Return	20	Percent/'Year
P.O. Period	0	Year

Table E- 2: Selective Parameters of Cash flow of first and second years of Acetic Acid Standalone Plant Part 1

CASHFLOW.ICS (Cashflow)	**Year**	**0**	**1**
ITEM	**UNITS**		
TW (Number of Weeks per Period)	Weeks/period	52	
T (Number of Periods for Analysis)	Period	20	
DTEPC (Duration of EPC Phase)	Period	0.519231	
DT (Duration of EPC Phase and Startup)	Period	0.903846	
WORKP (Working Capital Percentage)	Percent/period	5	
OPCHG (Operating Charges)	Percent/period	25	
PLANTOVH (Plant Overhead)	Percent/period	50	
CAPT (Total Project Cost)	Cost	1.49E+07	
RAWT (Total Raw Material Cost)	Cost/period	0	
PRODT (Total Product Sales)	Cost/period	0	
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.17E+06	
UTILT (Total Utilities Cost)	Cost/period	5.81E+06	
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20	
AF (ROR Annuity Factor)		5	
TAXR (Tax Rate)	Percent/period	40	
IF (ROR Interest Factor)		1.2	
ECONLIFE (Economic Life of Project)	Period	10	
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20	
DEPMETH (Depreciation Method)		Straight Line	
DEPMETHN (Depreciation Method Id)		1	
ESCAP (Project Capital Escalation)	Percent/period	5	
ESPROD (Products Escalation)	Percent/period	5	
ESRAW (Raw Material Escalation)	Percent/period	3.5	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3	
ESUT (Utilities Escalation)	Percent/period	3	
START (Start Period for Plant Startup)	Period	1	
PODE (Desired Payout Period (excluding EPC and Startup Phases))	Period		
POD (Desired Payout Period)	Period		
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5	
END (End Period for Economic Life of Project)	Period	10	
GA (G and A Expenses)	Percent/Period	8	
DTEP (Duration of EP Phase before Start of Construction)	Period	0.211538	
OP (Total Operating Labor Cost)	Cost/period	1.01E+06	
MT (Total Maintenance Cost)	Cost/period	165458	

Table E- 3: Selective Parameters of Cash flow of first and second years of Acetic Acid Standalone Plant Part 2

Expenses			
CASHFLOW.ICS (Cashflow)	**Year**	**0**	**1**
ITEM	**UNITS**		
CAP (Capital Costs)	Cost/Period	0	16444900.00
Unescalated Cumulative Capital Cost	Cost/Period	0	1.49E+07
Capital Cost	Cost/period	0	1.57E+07
Cumulative Capital Cost	Cost/period	0	1.57E+07
Working Capital	Cost/period		783,093.00
OP (Operating Costs)	Cost/Period	0	4.18E+06
Raw Materials	Cost/period	0	0
Operating Labor Cost	Cost/period	0	499198
Maintenance Cost	Cost/period	0	81933.7
Utilities	Cost/period	0	2.88E+06
Operating Charges	Cost/period	0	124800
Plant Overhead	Cost/period	0	290566
Subtotal Operating Costs	Cost/period	0	3.87E+06
G and A Costs	Cost/period	0	309755

Table E- 4: Equipment Costs of Acetic Acid Standalone Plant

Component Name	**Component Type**	**Total Direct Cost**	**Equipment Cost**
		(USD)	**(USD)**
EX-101	DHE TEMA EXCH	66700	10300
E106	DHE TEMA EXCH	66900	11500
TX-100-bottoms split	C	0	0
TX-100-cond	DHE TEMA EXCH	923300	606600
TX-100-cond acc	DHT HORIZ DRUM	108700	16100
TX-100-overhead split	C	0	0
TX-100-reb	DRB U TUBE	159900	62200
TX-100-reflux pump	DCP CENTRIF	49300	7500
TX-100-tower	DTW TOWER	1.10E+06	630500
PX-100	DCP CENTRIF	93600	54100
E107	DHE TEMA EXCH	64300	9900
RVX	DVT CYLINDER	170600	51700
E-104	DHE TEMA EXCH	183100	57500
E-113	DHE TEMA EXCH	79600	14400
E-114	DHE TEMA EXCH	522600	314700
EX-102	DHE TEMA EXCH	142700	40100
VX-100-flash vessel	DVT CYLINDER	147900	23300
MIX100	C	0	0
MAKEUPX	C	0	0
RECYCLEX	DVT CYLINDER	172500	23900
B4	C	0	0
EX-103	DHE TEMA EXCH	47500	7700
VLX-100	C	0	0
CX-100	DGC CENTRIF	1.30E+06	1.14E+06
E108	DHE TEMA EXCH	143200	45600
RX-100	DAT REACTOR	325200	166700
E-103	DHE TEMA EXCH	140200	39800
E-105	DHE TEMA EXCH	90200	19400
PX-101	DCP CENTRIF	73400	26200

Table E- 5: Utilities Cost Summary of Acetic Acid Standalone Plant

Description	Fluid	Item	Item Description	Rate, KWH	Units	Cost per Hour	Operating Pressure, PSAI	Operating Temperature, DEG F
Electricity		DCP CENTRIF	PX-100	44.76	KW	3.4689		
Electricity		DCP CENTRIF	PX-101	74.6	KW	5.7815		
Electricity		DCP CENTRIF	TX-100-reflux pump	18.65	KW	1.445375		
Electricity		DGC CENTRIF	CX-100	932.5	KW	72.26875		
Steam @100PSI	Steam	DRB U TUBE	TX-100-reb	27.115884	KLB	220.723296	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	EX-103	0.077389	KLB	0.629946	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	E-113	4.628377	KLB	37.674989	100	327.8
Steam @165PSI	Steam	DHE TEMA EXCH	EX-101	0.068409	KLB	0.667672	165	363.6
Steam @165PSI	Steam	DHE TEMA EXCH	E-104	13.76215	KLB	134.318584	165	363.6
Steam @165PSI	Steam	DHE TEMA EXCH	E-103	5.911643	KLB	57.697636	165	363.6
Steam @400PSI	Steam	DHE TEMA EXCH	EX-102	10.324334	KLB	120.897951	400	444.6

APPENDIX E.2 ECONOMICS SUMMARY OF ETHANOL STANDALONE PLANT

Table E- 6: Investment Summary for Ethanol Standalone Plant

INVESTMENT	Value	Units
Currency Conversion Rate	1	USD/U.S. DOLLAR
Total Project Capital Cost	3.45E+07	USD
Total Operating Cost	2.01E+07	USD/Year
Total Raw Materials Cost	0	USD/Year
Total Utilities Cost	1.53E+07	USD/Year
Total Product Sales	0	USD/Year
Desired Rate of Return	20	Percent/'Year
P.O. Period	0	Year

Table E- 7: Selective Parameters of Cash flow of first and second years of Ethanol Standalone Plant Part 1

CASHFLOW.ICS (Cashflow)	**Year**	**0**	**1**
ITEM	**UNITS**		
TW (Number of Weeks per Period)	Weeks/period	52	
T (Number of Periods for Analysis)	Period	20	
DTEPC (Duration of EPC Phase)	Period	0.730769	
DT (Duration of EPC Phase and Startup)	Period	1.11538	
WORKP (Working Capital Percentage)	Percent/period	5	
OPCHG (Operating Charges)	Percent/period	25	
PLANTOVH (Plant Overhead)	Percent/period	50	
CAPT (Total Project Cost)	Cost	3.45E+07	
RAWT (Total Raw Material Cost)	Cost/period	0	
PRODT (Total Product Sales)	Cost/period	0	
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.98E+06	
UTILT (Total Utilities Cost)	Cost/period	1.53E+07	
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20	
AF (ROR Annuity Factor)		5	
TAXR (Tax Rate)	Percent/period	40	
IF (ROR Interest Factor)		1.2	
ECONLIFE (Economic Life of Project)	Period	10	
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20	
DEPMETH (Depreciation Method)		Straight Line	
DEPMETHN (Depreciation Method Id)		1	
ESCAP (Project Capital Escalation)	Percent/period	5	
ESPROD (Products Escalation)	Percent/period	5	
ESRAW (Raw Material Escalation)	Percent/period	3.5	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3	
ESUT (Utilities Escalation)	Percent/period	3	
START (Start Period for Plant Startup)	Period	1	
PODE (Desired Payout Period (excluding EPC and Startup Phases))	Period		
POD (Desired Payout Period)	Period		
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5	
END (End Period for Economic Life of Project)	Period	10	
GA (G and A Expenses)	Percent/Period	8	
DTEP (Duration of EP Phase before Start of Construction)	Period	0.307692	
OP (Total Operating Labor Cost)	Cost/period	1.53E+06	
MT (Total Maintenance Cost)	Cost/period	450353	

Table E- 8: Selective Parameters of Cash flow of first and second years of Ethanol Standalone Plant Part 2

CASHFLOW.ICS (Cashflow)	**Year**	**0**	**1**
ITEM	**UNITS**		
Expenses			
CAP (Capital Costs)	Cost/Period	0	3.80E+07
Unescalated Cumulative Capital Cost	Cost/Period	0	3.45E+07
Capital Cost	Cost/period	0	3.62E+07
Cumulative Capital Cost	Cost/period	0	3.62E+07
Working Capital	Cost/period		1.81E+06
OP (Operating Costs)	Cost/Period	0	5.59E+06
Raw Materials	Cost/period	0	0
Operating Labor Cost	Cost/period	0	425404
Maintenance Cost	Cost/period	0	124886
Utilities	Cost/period	0	4.24E+06
Operating Charges	Cost/period	0	106351
Plant Overhead	Cost/period	0	275145
Subtotal Operating Costs	Cost/period	0	5.17E+06
G and A Costs	Cost/period	0	413851

Table E- 9: Equipment Costs of Ethanol Standalone Plant

Component Name	**Component Type**	**Total Direct Cost**	**Equipment Cost**
		(USD)	**(USD)**
E-104	DHE TEMA EXCH	56500	8400
T-100-bottoms split	C	0	0
T-100-cond	DHE TEMA EXCH	161100	59700
T-100-cond acc	DHT HORIZ DRUM	125600	23300
T-100-overhead split	C	0	0
T-100-reb	DRB U TUBE	114400	31100
T-100-reflux pump	DCP CENTRIF	52800	10200
T-100-tower	DTW TOWER	628000	320100
C123	DHE TEMA EXCH	153300	46800
C115	DHE TEMA EXCH	59700	8800
VL-100	C	0	0
B4	C	0	0
P-102	DCP CENTRIF	160600	98600
C112	DHE TEMA EXCH	97300	23900
RECYCLE	DVT CYLINDER	174800	55800
I104	DHE TEMA EXCH	79100	13800
C-100	DGC CENTRIF	1.15E+06	982000
R100V	DVT CYLINDER	198000	64200
V-100-flash vessel	DVT CYLINDER	152000	25200
P-200	DCP CENTRIF	33900	4700
P-201	DCP CENTRIF	32300	4600
R-100	DAT REACTOR	378600	210100
I113	DHE TEMA EXCH	158500	60300
I112	DHE TEMA EXCH	186200	62300
C-101	DGC CENTRIF	1.05E+06	894900
R-200	DAT REACTOR	228800	83600
H107	DHE TEMA EXCH	165700	64200
H110	DHE TEMA EXCH	105100	24100
H106	DHE TEMA EXCH	84800	16500
I116	DHE TEMA EXCH	307100	156800
MIX100	C	0	0
M-300	C	0	0
MAKEUP	C	0	0
P-100	DCP CENTRIF	102500	61900
I109	DHE TEMA EXCH	129700	32600
I103	DHE TEMA EXCH	351200	193000
E-105	DHE TEMA EXCH	157000	55800

Table E- 10: Utilities Cost Summary of Ethanol Standalone Plant

Description	Fluid	Item	Item Description	Rate, KWH	Units	Cost per Hour	Operating Pressure, PSIA	Operating Temperature, DEG F
Electricity		DCP CENTRIF	P-100	74.6	KW	5.7815		
Electricity		DCP CENTRIF	P-102	223.8	KW	17.3445		
Electricity		DCP CENTRIF	P-200	2.24	KW	0.1736		
Electricity		DCP CENTRIF	P-201	1.49	KW	0.115475		
Electricity		DCP CENTRIF	P-300	74.6	KW	5.7815		
Electricity		DCP CENTRIF	T-100-reflux pump	29.84	KW	2.3126		
Electricity		DCP CENTRIF	T-200-reflux pump	14.92	KW	1.1563		
Electricity		DCP CENTRIF	T-300-reflux pump	18.65	KW	1.445375		
Electricity		DCP CENTRIF	T-301-reflux pump	14.92	KW	1.1563		
Electricity		DGC CENTRIF	C-100	932.5	KW	72.26875		
Electricity		DGC CENTRIF	C-101	522.2	KW	40.4705		
Electricity		DGC CENTRIF	C-300	1865	KW	144.5375		
Electricity		DGC CENTRIF	C-301	2238	KW	173.445		
Cooling Water	Water	DHE TEMA EXCH	T-301-cond	0.242746	MMGAL	29.12952	50	95
Cooling Water	Water	DHE TEMA EXCH	T-300-cond	0.098063	MMGAL	11.76756	50	95
Cooling Water	Water	DHE TEMA EXCH	T-200-cond	0.121165	MMGAL	14.5398	50	95
Cooling Water	Water	DHE TEMA EXCH	T-100-cond	0.197248	MMGAL	23.66976	50	95
Cooling Water	Water	DHE TEMA EXCH	E-107	0.001097	MMGAL	0.13164	50	95
Cooling Water	Water	DHE TEMA EXCH	C115	0.002337	MMGAL	0.28044	50	95
Cooling Water	Water	DHE TEMA EXCH	C112	0.064845	MMGAL	7.7814	50	95
Refrigerant - Freon 12	Refrigerant	DHE TEMA EXCH	C123	219.812349	KLB	18.68405	15.5	-21.64
Steam @100PSI	Steam	DRB U TUBE	T-301-reb	66.609273	KLB	542.199482	100	327.8
Steam @100PSI	Steam	DRB U TUBE	T-300-reb	21.115343	KLB	171.878892	100	327.8
Steam @100PSI	Steam	DRB U TUBE	T-200-reb	1.014609	KLB	8.258917	100	327.8
Steam @100PSI	Steam	DRB U TUBE	T-100-reb	11.417486	KLB	92.938336	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	H-114	2.711015	KLB	22.067662	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	H-111	0.604731	KLB	4.92251	100	327.8
Steam @165PSI	Steam	DHE TEMA EXCH	H110	3.429946	KLB	33.476273	165	363.6
Steam @165PSI	Steam	DHE TEMA EXCH	H107	18.591576	KLB	181.453782	165	363.6
Steam @165PSI	Steam	DHE TEMA EXCH	E-105	3.300318	KLB	32.211104	165	363.6
Steam @165PSI	Steam	DHE TEMA EXCH	E-104	0.027519	KLB	0.268585	165	363.6

Steam @400PSI	Steam	DHE TEMA EXCH	H106	3.516077	KLB	41.173262	400	444.6
Steam @400PSI	Steam	DHE TEMA EXCH	E-300	5.458476	KLB	63.918754	400	444.6

APPENDIX E.3 ECONOMICS SUMMARY OF STRCTURALLY INTEGRATED PLANT

Table E- 11: Investment Summary for Structurally Integrated Plant

INVESTMENT	Value	Units
Currency Conversion Rate	1	USD/U.S. DOLLAR
Total Project Capital Cost	3.40E+07	USD
Total Operating Cost	2.39E+07	USD/Year
Total Utilities Cost	1.91E+07	USD/Year
Total Product Sales	0	USD/Year
Desired Rate of Return	20	Percent/'Year
P.O. Period	0	Year

Table E- 12: Selective Parameters of Cash flow of first and second years of Structurally Integrated Plant Part 1

CASHFLOW.ICS (Cashflow)	**Year**	**0**	**1**
ITEM	**UNITS**		
TW (Number of Weeks per Period)	Weeks/period	52	
T (Number of Periods for Analysis)	Period	20	
DTEPC (Duration of EPC Phase)	Period	0.730769	
DT (Duration of EPC Phase and Startup)	Period	1.11538	
WORKP (Working Capital Percentage)	Percent/period	5	
OPCHG (Operating Charges)	Percent/period	25	
PLANTOVH (Plant Overhead)	Percent/period	50	
CAPT (Total Project Cost)	Cost	3.40E+07	
RAWT (Total Raw Material Cost)	Cost/period	0	
PRODT (Total Product Sales)	Cost/period	0	
OPMT (Total Operating Labor and Maintenance Cost)	Cost/period	1.81E+06	
UTILT (Total Utilities Cost)	Cost/period	1.91E+07	
ROR (Desired Rate of Return/Interest Rate)	Percent/period	20	
AF (ROR Annuity Factor)		5	
TAXR (Tax Rate)	Percent/period	40	
IF (ROR Interest Factor)		1.2	
ECONLIFE (Economic Life of Project)	Period	10	
SALVAL (Salvage Value (Percent of Initial Capital Cost))	Percent	20	
DEPMETH (Depreciation Method)		Straight Line	
DEPMETHN (Depreciation Method Id)		1	
ESCAP (Project Capital Escalation)	Percent/period	5	
ESPROD (Products Escalation)	Percent/period	5	
ESRAW (Raw Material Escalation)	Percent/period	3.5	
ESLAB (Operating and Maintenance Labor Escalation)	Percent/period	3	
ESUT (Utilities Escalation)	Percent/period	3	
START (Start Period for Plant Startup)	Period	1	
PODE (Desired Payout Period (excluding EPC and Startup Phases))	Period		
POD (Desired Payout Period)	Period		
DESRET (Desired Return on Project for Sales Forecasting)	Percent/Period	10.5	
END (End Period for Economic Life of Project)	Period	10	
GA (G and A Expenses)	Percent/Period	8	
DTEP (Duration of EP Phase before Start of Construction)	Period	0.288462	
OP (Total Operating Labor Cost)	Cost/period	1.36E+06	
MT (Total Maintenance Cost)	Cost/period	455832	

Table E- 13: Selective Parameters of Cash flow of first and second years of Structurally Integrated Plant Part 2

CASHFLOW.ICS (Cashflow)	**Year**	**0**	**1**
Expenses			
CAP (Capital Costs)	Cost/Period	0	3.74E+07
Unescalated Cumulative Capital Cost	Cost/Period	0	3.40E+07
Capital Cost	Cost/period	0	3.56E+07
Cumulative Capital Cost	Cost/period	0	3.56E+07
Working Capital	Cost/period		1.78E+06
OP (Operating Costs)	Cost/Period	0	6.64E+06
Raw Materials	Cost/period	0	0
Operating Labor Cost	Cost/period	0	376786
Maintenance Cost	Cost/period	0	126406
Utilities	Cost/period	0	5.30E+06
Operating Charges	Cost/period	0	94196.6
Plant Overhead	Cost/period	0	251596
Subtotal Operating Costs	Cost/period	0	6.15E+06
G and A Costs	Cost/period	0	491880

Table E- 14: Equipment Costs of Structurally Integrated Plant Part 1

Component Name	**Component Type**	**Total Direct Cost**
		(USD)
EX-101	DHE TEMA EXCH	68000
MAKEUPX	C	0
B1	C	0
CX-100	DGC CENTRIF	1.39E+06
MIX100	C	0
E-200	DHE TEMA EXCH	64400
EX-102	DHE TEMA EXCH	156900
B4	C	0
P-201	DCP CENTRIF	38000
R-100	DAT REACTOR	389100
P-200	DCP CENTRIF	38200
R-200	DAT REACTOR	228200
PX-101	DCP CENTRIF	78300
B9	C	0
V-100-flash vessel	DVT CYLINDER	151900
T-200-bottoms split	C	0
T-200-cond	DHE TEMA EXCH	230000
T-200-cond acc	DHT HORIZ DRUM	150700
T-200-overhead split	C	0
T-200-reb	DRB U TUBE	96800
T-200-reflux pump	DCP CENTRIF	55700
T-200-tower	DTW TOWER	912000
T-100-bottoms split	C	0
T-100-cond	DHE TEMA EXCH	158400
T-100-cond acc	DHT HORIZ DRUM	113700
T-100-overhead split	C	0
T-100-reb	DRB U TUBE	197200
T-100-reflux pump	DCP CENTRIF	51900
T-100-tower	DTW TOWER	1.32E+06
RECYCLEX	DVT CYLINDER	166300
B2	DCP CENTRIF	100100
RVX	DVT CYLINDER	203500
VLX-100	C	0

Table E- 15: Equipment Cost of Structurally Integrated Plant Part 2

Component Name	**Component Type**	**Total Direct Cost**
		(USD)
C-301	DGC CENTRIF	1.86E+06
C-300	DGC CENTRIF	1.80E+06
R-300	DAT REACTOR	290500
V-300-flash vessel	DVT CYLINDER	142500
E-301	DHE TEMA EXCH	65400
VL-300	C	0
T-300-bottoms split	C	0
T-300-cond	DHE TEMA EXCH	189300
T-300-cond acc	DHT HORIZ DRUM	148300
T-300-overhead split	C	0
T-300-reb	DRB U TUBE	205100
T-300-reflux pump	DCP CENTRIF	49700
T-300-tower	DTW TOWER	1.20E+06
I122	DHE TEMA EXCH	75100
I118	DHE TEMA EXCH	265900
C132	DHE TEMA EXCH	139900
B17	C	0
H119	DHE TEMA EXCH	98500
B11	C	0
I125	DHE TEMA EXCH	77600
B12	C	0
I112	DHE TEMA EXCH	64900
H117	DHE TEMA EXCH	134500
C129	DHE TEMA EXCH	124700
C111	DHE TEMA EXCH	74000
C115	DHE TEMA EXCH	220600
I121	DHE TEMA EXCH	139800
C120	DHE TEMA EXCH	118800
H108	DHE TEMA EXCH	108100
I107	DHE TEMA EXCH	318300
H110	DHE TEMA EXCH	199900
P-300	DCP CENTRIF	101200
E-300	DHE TEMA EXCH	108200
H131	DHE TEMA EXCH	84100
I116	DHE TEMA EXCH	354300
H109	DHE TEMA EXCH	64300

Table E- 16: Utilities Cost Summary of Structurally Integrated Plant

Description	Fluid	Item	Item Description	Rate, KWH	Units	Cost per Hour	Operating Pressure, PSIA	Operating Temperature, DEG F
Electricity		DCP CENTRIF	B2	74.6	KW	5.7815		
Electricity		DCP CENTRIF	P-200	3.73	KW	0.289075		
Electricity		DCP CENTRIF	P-201	3.73	KW	0.289075		
Electricity		DCP CENTRIF	P-300	74.6	KW	5.7815		
Electricity		DCP CENTRIF	PX-101	93.25	KW	7.226875		
Electricity		DCP CENTRIF	T-100-reflux pump	29.84	KW	2.3126		
Electricity		DCP CENTRIF	T-200-reflux pump	29.84	KW	2.3126		
Electricity		DCP CENTRIF	T-300-reflux pump	14.92	KW	1.1563		
Electricity		DGC CENTRIF	C-300	1865	KW	144.5375		
Electricity		DGC CENTRIF	C-301	2238	KW	173.445		
Electricity		DGC CENTRIF	CX-100	1492	KW	115.63		
Cooling Water	Water	DHE TEMA EXCH	T-300-cond	0.24621	MMGAL	29.5452	50	95
Cooling Water	Water	DHE TEMA EXCH	T-200-cond	0.218265	MMGAL	26.1918	50	95
Cooling Water	Water	DHE TEMA EXCH	T-100-cond	0.217269	MMGAL	26.07228	50	95
Cooling Water	Water	DHE TEMA EXCH	C129	0.07628	MMGAL	9.1536	50	95
Cooling Water	Water	DHE TEMA EXCH	C120	0.165213	MMGAL	19.82556	50	95
Cooling Water	Water	DHE TEMA EXCH	C111	0.042903	MMGAL	5.14836	50	95
Refrigerant - Freon 12	Refrigerant	DHE TEMA EXCH	C132	152.400397	KLB	12.954034	15.5	-21.64
Steam @100PSI	Steam	DRB U TUBE	T-300-reb	67.508712	KLB	549.520916	100	327.8
Steam @100PSI	Steam	DRB U TUBE	T-200-reb	9.460175	KLB	77.005825	100	327.8
Steam @100PSI	Steam	DRB U TUBE	T-100-reb	41.125377	KLB	334.760569	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	H131	3.957092	KLB	32.210729	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	H119	12.608961	KLB	102.636943	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	H117	5.712741	KLB	46.501712	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	H109	0.569925	KLB	4.63919	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	E-301	0.942348	KLB	7.670713	100	327.8
Steam @100PSI	Steam	DHE TEMA EXCH	E-200	0.658854	KLB	5.363072	100	327.8
Steam @165PSI	Steam	DHE TEMA EXCH	H110	10.563983	KLB	103.104474	165	363.6
Steam @165PSI	Steam	DHE TEMA EXCH	EX-101	0.106889	KLB	1.043237	165	363.6
Steam @400PSI	Steam	DHE TEMA EXCH	H108	7.411936	KLB	86.793771	400	444.6
Steam @400PSI	Steam	DHE TEMA EXCH	EX-102	16.131772	KLB	188.90305	400	444.6

Steam @400PSI	Steam	DHE TEMA EXCH	E-300	5.633114	KLB	65.963765	400	444.6

APPENDIX F

HEAT INTEGRATION DATA OF SIMULATED PLANTS

APPENDIX F.1 HEAT INTEGRATION DATA OF ACETIC ACID STANDALONE PLANT

Table F- 1: Heat Exchanger Network Design Specifications of Acetic Acid Plant Part 1

Heat Exchanger	Type	Hot Stream	Hot T in, C	Hot T out, C	Cold Stream
E-103	Heater	HP Steam	250	249.4	SX-100_To_SX-101
E-104	Heater	HP Steam	250	249.4	SX-109_To_SX-110
E-105	Cooler	SX-115_To_SX-116	131.32	124.1	Air
E-106	Process	SX-115_To_SX-116	124.1	123.38	SX-100_To_SX-101
E-107	Process	SX-115_To_SX-116	123.38	118.75	SX-109_To_SX-110
E-108	Process	SX-115_To_SX-116	118.75	114.8	SX-100_To_SX-101
E-109	Cooler	H-R100	180	179.5	LP Steam Generation
E-110	Heater	LP Steam	125	124	SX-107_To_SX-108
E-111	Heater	HP Steam	249.4	249	SX-102_To_SX-103
E-112	Heater	HP Steam	249.4	249	SX-111_To_SX-112
E-113	Cooler	SX-115_To_SX-116	114.8	110.99	Air
E-114	Cooler	SX-115_To_SX-116	110.99	89.11	Air

Table F- 2: Heat Exchanger Network Design Specifications of Acetic Acid Plant Part 2

Heat Exchanger	Type	Cold T in,, C	Cold T out, C	dT Min Hot, C	dT Min Cold, C
E-103	Heater	117.3	180	70	132.1
E-104	Heater	117.3	180	70	132.1
E-105	Cooler	30	30.42	100.9	94.1
E-106	Process	115.5	117.3	6.81	7.88
E-107	Process	75.39	117.3	6.08	43.36
E-108	Process	26.69	115.5	3.25	88.11
E-109	Cooler	124	125	55	55.5
E-110	Heater	73.58	74.26	50.74	50.42
E-111	Heater	177.25	180	69.4	71.75
E-112	Heater	180	210.7	38.7	69
E-113	Cooler	33.66	35	79.8	77.33
E-114	Cooler	30.42	33.66	77.33	58.69

APPENDIX F.2 HEAT INTEGRATION DATA OF ETHANOL STANDALONE PLANT

Table F- 3: Heat Exchanger Network Design Specifications of Ethanol Plant Part 1

Heat Exchanger	Type	Load, kJ/h	Cost Index, [Cost]	Area, m2	Shells	LMTD, C
E-108	Cooler	2,090,254.80	55748.88	157.26	1	34.99
E-110	Heater	3,138,558.17	13300.66	5.88	1	102.57
E-109	Process	681,547.08	24259.81	36.63	1	23.74
E-105	Process	10,511,755.49	181340.6	688.98	2	42.38
E-107	Heater	15,340,205.33	67152.75	207.7	1	106.06
E-116	Process	8,515,550.10	281891.7	1031.85	4	14.98
E-118	Cooler	41,052,239.04	319473.3	1303.58	3	45.2
E-104	Process	628,432.33	29528.3	54.26	1	56.15
E-106	Heater	2,605,691.46	14133.07	7.79	1	64.22
E-123	Cooler	16,816,914.37	43131.18	105.06	1	57.29
E-113	Process	3,743,764.67	37334.36	69.47	2	19.83
E-111	Heater	616,905.37	10916.4	1.19	1	95.84
E-115	Cooler	717,174.09	28592.02	51.03	1	72.22
E-119	Heater	68,230.27	11449.08	2.1	1	80.5
E-117	Process	1,558,911.76	30506.91	57.68	1	75.08
E-121	Heater	4,579,413.02	46311.04	117.81	1	69.62
E-103	Process	7,089,267.31	86638.25	252.02	2	45.16
E-122	Cooler	11,346,949.37	142881.6	501.43	2	58.6
E-114	Heater	2,916,695.01	12884.65	4.97	1	121.9
E-112	Process	6,167,663.63	82461.58	234.97	2	42.34
E-120	Heater	2,989,365.52	30587.27	57.96	1	74.03

Table F- 4: Heat Exchanger Network Design Specifications of Ethanol Plant Part 2

Heat Exchanger	Type	Overall U, kJ/h.m2.C	Ffactor	Hot Stream	Hot T in, C	Hot T out, C
E-108	Cooler	378.92	1	S-111_To_S9	70.21	60.85
E-110	Heater	5204.23	1	HP Steam	249.38	249.27
E-109	Process	806.04	0.97	S10_To_S11	147.93	142.87
E-105	Process	360	1	HR1	170	169.9
E-107	Heater	696.77	1	HP Steam	250	249.38
E-116	Process	640.2	0.83	S10_To_S11	119.7	106.16
E-118	Cooler	696.77	1	HR1	169.9	169.5
E-104	Process	208.12	0.99	S-102_To_S-103	148.68	122.83
E-106	Heater	5213.41	1	HP Steam	250	249.38
E-123	Cooler	2715.48	1	S10_To_S11	78.15	3
E-113	Process	2880.23	0.95	S10_To_S11	124.73	119.7
E-111	Heater	5431.46	1	MP Steam	175	174.83
E-115	Cooler	194.65	1	S-102_To_S-103	122.83	93.33
E-119	Heater	403.34	1	HP Steam	249.27	249
E-117	Process	360	1	HR3	200	199.5
E-121	Heater	558.56	1	HP Steam	249.27	249
E-103	Process	801.28	0.81	S10_To_S11	200	147.93
E-122	Cooler	381.35	0.99	S10_To_S11	106.16	78.15
E-114	Heater	4817.58	1	MP Steam	174.83	174
E-112	Process	915.47	0.9	S10_To_S11	142.87	124.73
E-120	Heater	696.77	1	HP Steam	249.27	249

Table F- 5: Heat Exchanger Network Design Specifications of Ethanol Plant Part 3

Heat Exchanger	Type	Cold stream	Cold T, C	Cold T out, C	dT min Hot, C	dT min Cold, C
E-108	Cooler	Air	30	30.74	39.47	30.85
E-110	Heater	S1_To_S21	121.48	168.46	80.91	127.79
E-109	Process	S-201_To_S-202	112.17	130	17.93	30.7
E-105	Process	R-200_heat	125.04	130	40	44.86
E-107	Heater	S-113_To_S-114	112.14	170	80	137.24
E-116	Process	S-113_To_S-114	80.02	112.14	7.57	26.14
E-118	Cooler	LP Steam Generation	124	125	44.9	45.5
E-104	Process	S6_To_S7	75.87	82.22	66.45	46.96
E-106	Heater	S1_To_S21	168.46	200	50	80.91
E-123	Cooler	Refrigerant 1	-25	-24	102.15	28
E-113	Process	S1_To_S21	58.09	121.48	3.25	61.61
E-111	Heater	S-100_To_S-101	74.82	83.2	91.8	100.01
E-115	Cooler	Air	34.75	35	87.83	58.59
E-119	Heater	S-104_To_S-105	167.25	170	79.27	81.75
E-117	Process	R-200_heat	124.3	125.04	74.96	75.2
E-121	Heater	S8_To_S2	154.07	200	49.27	94.93
E-103	Process	S-100_To_S-101	83.2	170	30	64.73
E-122	Cooler	Air	30.74	34.75	71.41	47.41
E-114	Heater	S-100_To_S-101	27.23	74.82	100.01	146.77
E-112	Process	S-203_To_S-204	25.29	130	12.87	99.44
E-120	Heater	S-106_To_S-107	170	180	69.27	79

APPENDIX F.3 HEAT INTEGRATION DATA OF STRUCTURALLY INTGERATED PLANT

Table F- 6: The Design Specifications of the Heat Exchanger Network for Structurally Integrated Plant Part 1

Heat Exchanger	Type	Load, kJ/h	Cost Index, [Cost]	Area, m2	Shells	LMTD, C	Overall U, kJ/h.m2.C	Ffactor	Hot Stream
E-107	Process	3140150.70	85032.07	245.44	2	20.05	803.36	0.79	S10_To_S11
E-108	Heater	5853840.85	16520.36	13.77	1	83.21	5243.02	1.00	HP Steam
E-109	Heater	580855.93	26185.45	42.91	1	130.10	104.06	1.00	HP Steam
E-110	Heater	7167258.75	46263.28	117.62	1	87.48	696.77	1.00	HP Steam
E-111	Cooler	12291788.43	114606.84	442.17	1	93.69	308.29	1.00	SX-115_To_QS7
E-112	Process	13051078.65	104349.39	388.65	1	9.93	2676.83	0.89	SX-115_To_QS7
E-113	Process	1451591.68	30483.25	57.60	1	70.01	360.00	1.00	R-300_heat
E-114	Cooler	125811051.75	774653.36	3267.34	7	55.26	696.77	1.00	B3_heat
E-115	Cooler	3812723.38	46948.08	120.40	1	36.95	858.90	1.00	S10_To_S11
E-116	Process	12566147.72	822437.94	3309.90	9	19.73	502.37	0.82	S10_To_S11
E-117	Heater	5465410.05	21560.67	28.18	1	34.83	5728.31	0.99	MP Steam
E-118	Process	8733262.60	61425.73	138.30	3	23.13	3183.72	0.90	S10_To_S11
E-119	Heater	235354.36	10294.27	0.29	1	152.32	5394.03	1.00	HP Steam
E-120	Cooler	11769389.44	115595.32	447.40	1	68.84	377.20	1.00	SX-115_To_QS7
E-121	Process	2182428.86	21552.10	23.67	2	26.73	3745.73	0.95	S10_To_S11
E-122	Process	3321235.20	62742.50	187.86	1	27.84	651.86	0.97	SX-115_To_QS7
E-123	Heater	628107.08	16851.92	14.65	1	95.01	451.19	1.00	MP Steam
E-124	Heater	616430.08	11742.60	2.65	1	49.89	4669.95	1.00	MP Steam
E-125	Process	393724.27	11441.79	2.09	1	58.43	3228.24	1.00	SX-115_To_QS7
E-126	Heater	4579151.74	46213.93	117.42	1	69.88	558.53	1.00	HP Steam
E-127	Heater	96818.05	12572.97	4.31	1	70.73	317.84	1.00	HP Steam
E-128	Heater	13282567.19	99325.23	362.96	1	52.57	696.77	1.00	HP Steam
E-129	Cooler	12430984.53	186136.16	713.17	2	44.00	380.17	0.99	S10_To_S11
E-130	Process	7833433.95	110988.87	423.14	1	51.42	360.00	1.00	B3_heat
E-131	Heater	3775942.87	12763.96	4.71	1	157.57	5087.71	1.00	HP Steam
E-132	Cooler	11776944.25	38359.94	86.50	1	50.89	2685.90	1.00	S10_To_S11

Table F- 7: The Design Specifications of the Heat Exchanger Network for Structurally Integrated Plant Part 2

Heat Exchanger	Type	Hot T in, C	Hot T out, C	Cold stream	Cold T, C	Cold T out, C	dT min Hot, C	dT min Cold, C
E-107	Process	200.00	177.11	SX-100_To_SX-101	157.02	180.00	20.00	20.09
E-108	Heater	250.00	249.62	S1_To_S21	120.99	200.00	50.00	128.63
E-109	Heater	250.00	249.62	S-203_To_S-204	108.86	130.00	120.00	140.75
E-110	Heater	250.00	249.62	SX-109_To_SX-110	141.96	180.00	70.00	107.66
E-111	Cooler	131.32	117.99	Air	30.00	31.68	99.63	87.99
E-112	Process	117.99	110.99	S-203_To_S-204	100.20	108.86	9.12	10.79
E-113	Process	200.00	199.50	R-200_heat	129.48	130.00	70.00	70.02
E-114	Cooler	180.00	179.53	LP Steam Generation	124.00	125.00	55.00	55.53
E-115	Cooler	177.11	149.06	LP Steam Generation	124.00	125.00	52.11	25.06
E-116	Process	149.06	117.54	SX-109_To_SX-110	75.25	141.96	7.11	42.28
E-117	Heater	175.00	174.19	SX-100_To_SX-101	114.29	157.02	17.98	59.90
E-118	Process	117.54	102.71	SX-100_To_SX-101	26.46	114.29	3.25	76.25
E-119	Heater	249.62	249.61	S-203_To_S-204	94.36	100.20	149.42	155.25
E-120	Cooler	110.99	95.55	Air	33.39	35.00	75.99	62.16
E-121	Process	102.71	98.43	S-203_To_S-204	36.54	94.36	8.35	61.89
E-122	Process	95.55	89.79	SX-107_To_SX-108	54.19	74.26	21.29	35.60
E-123	Heater	174.19	174.00	S6_To_S7	75.87	82.22	91.96	98.13
E-124	Heater	174.19	174.00	S-201_To_S-202	117.94	130.00	44.19	56.06
E-125	Process	89.79	89.11	S-203_To_S-204	25.18	36.54	53.25	63.93
E-126	Heater	249.61	249.11	S8_To_S2	154.07	200.00	49.61	95.04
E-127	Heater	249.61	249.11	SX-102_To_SX-103	177.25	180.00	69.61	71.86
E-128	Heater	249.61	249.11	SX-111_To_SX-112	180.00	210.70	38.91	69.11
E-129	Cooler	98.43	59.76	Air	31.68	33.39	65.05	28.08
E-130	Process	179.53	179.50	R-200_heat	126.67	129.48	50.05	52.83
E-131	Heater	249.11	249.00	S1_To_S21	57.78	120.99	128.12	191.22
E-132	Cooler	59.76	3	Refrigerant 1	-25	-24	83.76	28